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Poly[di-μ_3-chloro-μ_2-4,4′-bipyridine-dicopper(I)]

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The structure of the title compound, $[Cu_2Cl_2(C_{10}H_8N_2)]_n$, consists of a two-dimensional layer. Each Cl atom bridges three Cu atoms to form a ladder-like structure, whereas the 4,4′-bipyridine ligands form a link between Cu atoms of adjacent ladders, thus building a two-dimensional layer structure.

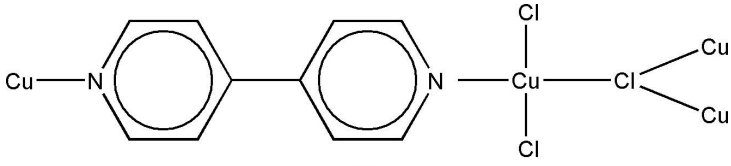
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.037
wR factor = 0.089
Data-to-parameter ratio = 15.0

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

Comment

Research in metal–organic coordination polymers is rapidly expanding, because of their fascinating structural diversity and potential applications as functional materials (Eddaoudi *et al.*, 2000; Li *et al.*, 1998; Moulton & Zaworokto, 2001). 4,4′-Bipyridine (4,4′-bpy), as a neutral bridging ligand, is widely used to construct porous coordination polymers with transition metal ions, due to its rodlike rigidity and favourable linearity. In this paper, we report the synthesis and structure of the title complex, $[Cu_2Cl_2(bpy)]_n$, (I).



(I)

Each Cu^I ion is coordinated by three Cl atoms and by one N atom from a bipy ligand, and has a tetrahedral geometry (Fig. 1).

All Cl atoms link to three Cu metal centres, with Cu—Cl distances varying from 2.3025 (12) to 2.4959 (15) Å, forming a ladder-like structure. Adjacent pairs of ladders are joined by 4,4′-bpy molecules *via* their two N-atom sites, leading to a two-dimensional layer structure containing regular parallelogram grids along the *c* axis (Fig. 2).

Experimental

A mixture of $GdCl_3{\cdot}6H_2O$ (0.1 mmol), $CuCl_2{\cdot}2H_2O$ (0.2 mmol), 2-aminoterephthalic acid (0.2 mmol), 4,4′-bipyridine (0.2 mmol), water (6 ml), *n*-propanol (6 ml) and 0.65 *M* NaOH aqueous solution (0.65 ml, 0.42 mmol) was sealed in a 25 ml Teflon-lined stainless steel reactor and heated at 433 K for 72 h under autogeneous pressure, then cooled to 373 K at a rate of 10 K every 3 h, followed by slow cooling to room temperature. Upon cooling to room temperature, two kinds of crystals were obtained. The majority were brown block-shaped crystals of (I) and the minority were tiny yellow crystals, which have previously been reported by us (Liu *et al.*, 2005). Analysis,

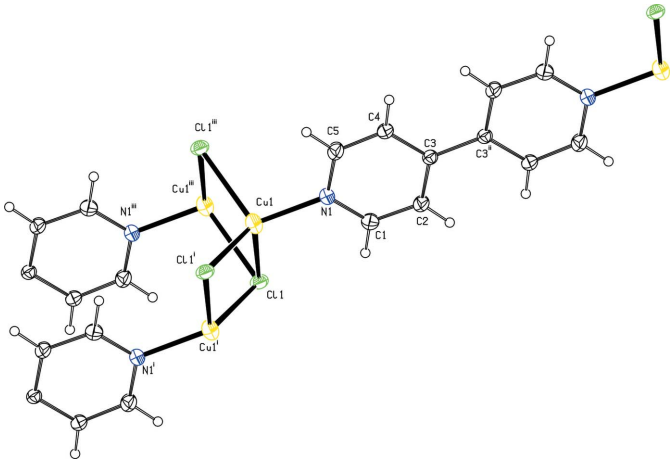


Figure 1
Part of the polymeric structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as spheres of arbitrary radii. [Symmetry codes: (i) $-x, 1-y, -z$; (ii) $1-x, -y, -z$; (iii) $1-x, 1-y, -z$.]

calculated for C_5H_4ClNCu (177.1): C 33.88, H 2.26, N 7.91%; found: C 33.98, H 2.08, N 8.09%.

Crystal data

$[Cu_2Cl_2(C_{10}H_8N_2)]$	$Z = 4$
$M_r = 177.09$	$D_x = 2.129$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 3.7853$ (19) Å	$\mu = 4.30$ mm^{-1}
$b = 12.732$ (6) Å	$T = 293$ (2) K
$c = 11.505$ (6) Å	Block, brown
$\beta = 94.748$ (8)°	0.20 × 0.20 × 0.18 mm
$V = 552.6$ (5) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3033 measured reflections
φ and ω scans	1093 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	957 reflections with $I > 2\sigma(I)$
$T_{min} = 0.424$, $T_{max} = 0.476$	$R_{int} = 0.041$
	$\theta_{max} = 26.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0325P)^2 + 0.7193P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.037$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.089$	$\Delta\rho_{max} = 0.47$ e Å^{-3}
$S = 1.17$	$\Delta\rho_{min} = -0.82$ e Å^{-3}
1093 reflections	
73 parameters	
H-atom parameters constrained	

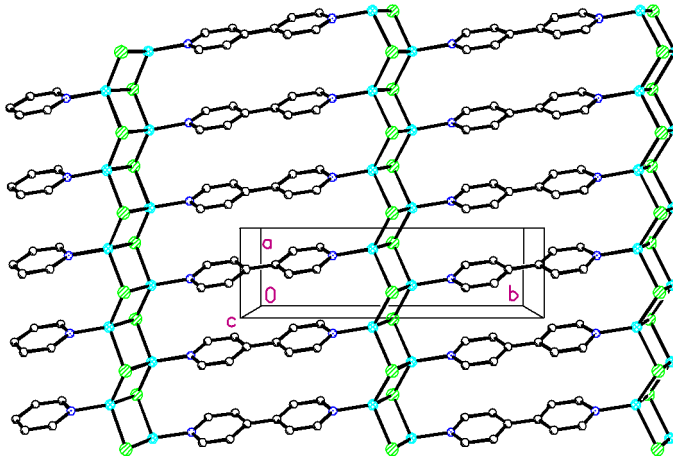


Figure 2
A packing diagram for (I), viewed along the *c* axis. All H atoms have been omitted for clarity.

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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, 1998) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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