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Poly[[μ-2-amino-4-(2-pyridyl)-6-(4-pyridyl)-pyrimidine-$\kappa^3N,N':N''$]di-μ-bromido-dicopper(I)]

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.009 Å
R factor = 0.048
wR factor = 0.139
Data-to-parameter ratio = 12.8

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

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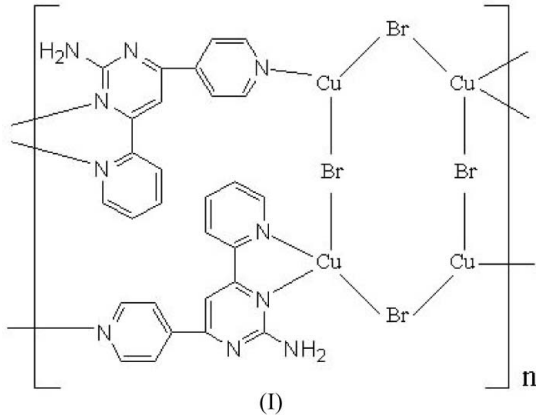
In the title complex, $[Cu_2Br_2(C_{14}H_{11}N_5)]_n$, there are two crystallographically independent Cu^I cations with different coordination geometries: one has tetrahedral geometry ($CuBr_2N_2$), and the other adopts a trigonal geometry ($CuBr_2N$). The 2-amino-4-(2-pyridyl)-6-(4-pyridyl)pyrimidine (appm) ligand acts as a bridging ligand. Four Br^- anions connect four Cu^I cations to form an eight-membered ring, and the appm ligands link adjacent eight-membered rings to construct a one-dimensional ribbon chain.

Comment

In order to obtain novel structural motifs with predictable properties, a large number of organic ligands have been designed and utilized (Bu *et al.*, 2002). Among them, there is increasing interest in *N*,*N*′-chelating ligands, especially *N*,*N*′-chelating oligopyridine ligands (Patroniak *et al.*, 2005; Petitjean *et al.*, 2004). During investigation of the coordination chemistry of *N*,*N*′-chelating oligopyridine ligands, our attention was attracted by the 2-amino-4-(2-pyridyl)-6-(4-pyridyl)-pyrimidine (appm) ligand. The coordination chemistry of appm has not been widely explored, except for one Ag^I compound recently reported by us (Chi *et al.*, 2006). We report here the structure of the title Cu^I complex, (I), formed by the reaction of $CuBr_2$ and 2-amino-4-(2-pyridyl)-6-(4-pyridyl)-pyrimidine under hydrothermal conditions.



(I)

The title polymer consists of a one-dimensional ribbon chain (Figs. 1 and 2). There are two crystallographically independent Cu^I cations with different coordination geometries, one with a distorted tetrahedral $CuBr_2N_2$ geometry (Table 1) and the other with a distorted trigonal $CuBr_2N$ geometry.

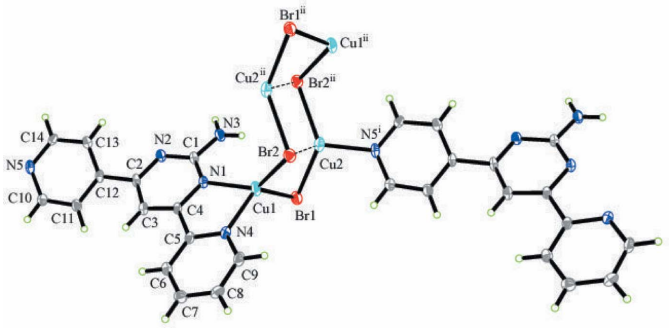


Figure 1
A part of the polymeric structure of (I), with 30% probability displacement ellipsoids. Dashed lines represent weak interactions between atoms Cu2 and Br2. [Symmetry codes: (i) $x-1, y, z+1$; (ii) $-x+1, -y, -z+1$.]

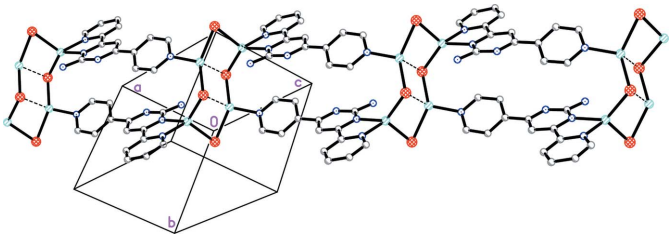


Figure 2
The one-dimensional chain structure of (I). Dashed lines represent weak interactions between atoms Cu2 and Br2. H atoms have been omitted for clarity.

The Cu2···Br2 separation of 2.756 (1) Å indicates a weak interaction. Each Br^- anion exhibits a μ_2-bridging coordination mode. Four Br^- anions connect four Cu^I cations to form an eight-membered ring. In this ring, the distance between atoms Cu1 and Cu2 is 2.848 (1) Å. The appm ligands bridge adjacent eight-membered rings to form a one-dimensional ribbon chain (Fig. 2).

Experimental

A mixture of the appm ligand (24.9 mg, 0.1 mmol), $CuBr_2$ (22.3 mg, 0.1 mmol) and H_2O (8 ml) was transferred to and sealed in a 15 ml Teflon-lined stainless steel container. The container was heated to 433 K for 72 h, and then cooled to room temperature. Single crystals of (I) were obtained (yield 18.76 mg, *ca* 35% based on the ligand appm). Elemental analysis, calculated for $C_{14}H_{11}Br_2Cu_2N_5$: C 31.33, H 2.05, N 13.06%; found: C 31.41, H 2.11, N 13.01%.

Crystal data

$[Cu_2Br_2(C_{14}H_{11}N_5)]$
$M_r = 536.18$
Triclinic, $P\overline{1}$
$a = 7.495$ (2) Å
$b = 9.998$ (3) Å
$c = 11.384$ (4) Å
$\alpha = 71.699$ (4)°
$\beta = 84.631$ (5)°
$\gamma = 71.660$ (4)°
$V = 768.7$ (4) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 7.97$ mm^{-1}
$T = 298$ (2) K
0.48 × 0.18 × 0.08 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.106$, $T_{max} = 0.530$
4013 measured reflections
2660 independent reflections
2126 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.139$
$S = 1.00$
2660 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.97$ e Å^{-3}
$\Delta\rho_{min} = -1.10$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.085 (5)	Cu2—N5^{i}	2.019 (5)
Cu1—N4	2.069 (5)	Cu2—Br1	2.449 (1)
Cu1—Br1	2.460 (1)	Cu2···Br2	2.756 (1)
Cu1—Br2	2.446 (1)	Cu2—Br2^{ii}	2.428 (1)
Cu1···Cu2	2.848 (1)		
N4—Cu1—N1	78.72 (18)	N5^{i}—Cu2—Br2^{ii}	115.83 (16)
N1—Cu1—Br2	132.84 (14)	N5^{i}—Cu2—Br1	105.96 (16)
N4—Cu1—Br1	123.48 (14)	Br2^{ii}—Cu2—Br1	125.57 (5)
Br2—Cu1—Br1	111.42 (4)		

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

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C), and with N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; 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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