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Key indicators

Single-crystal X-ray study

$T = 292$ K

Mean $\sigma(C-C) = 0.010$ Å

R factor = 0.079

wR factor = 0.213

Data-to-parameter ratio = 15.4

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

Hydrothermal synthesis of a copper(I) stair-like polymer: *catena*-poly[[bis[5-(4-bromophenyl)-2-(4-pyrimidyl)pyridine]-dicopper(I)]-di- μ_3 -bromo]

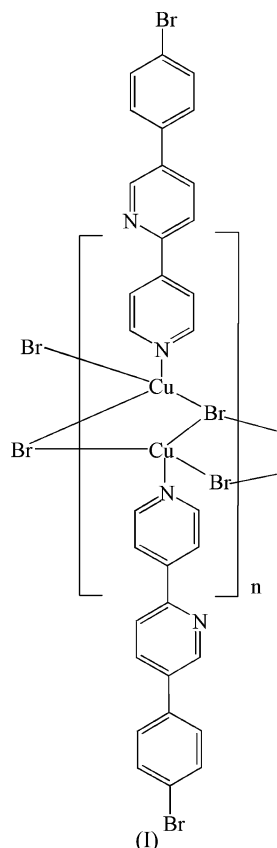
In the title compound, $[\text{Cu}_2\text{Br}_2(\text{C}_{16}\text{H}_{11}\text{BrN}_2)_2]_n$, each Cu atom displays a distorted tetrahedral coordination formed by three Br atoms and one N atom from 5-(4-bromophenyl)-2-(4-pyrimidyl)pyridine. Each Br atom bridges three Cu atoms, forming a stair-like structure along the b axis.

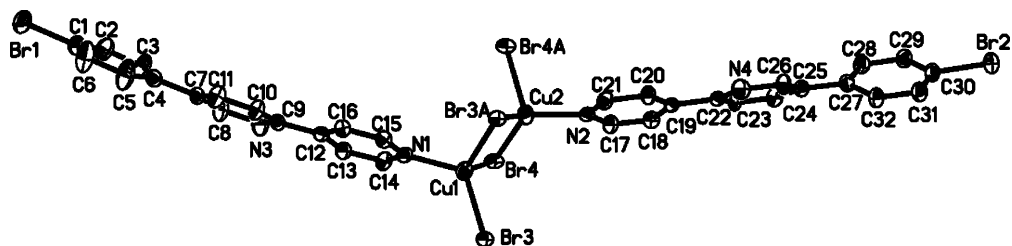
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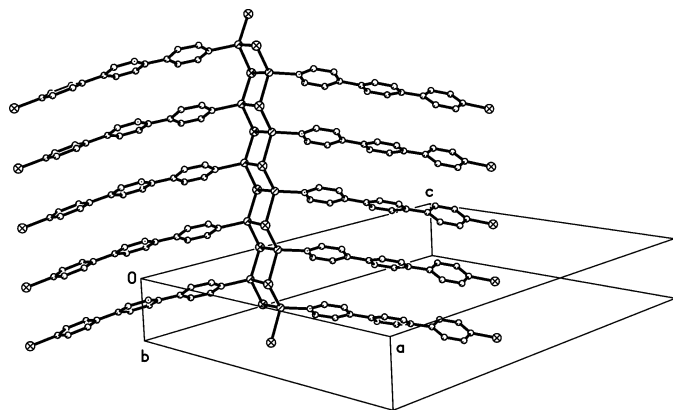
Comment

A remarkable series of copper(I) halides has been investigated due to their rich photophysical properties (Ford *et al.*, 1999). Previously, the most quantitative photophysical study has focused on copper(I) tetranuclear complexes (Ryu *et al.*, 1993). In recent years, much interest has been paid to other multinuclear copper(I) halide complexes with aromatic nitrogen-donor ligands (Ohi *et al.*, 2005; Wang *et al.*, 2005). As part of our research, we chose the conjugated 5-(4-bromophenyl)-2-(4-pyrimidyl)pyridine (bppy) molecule as a pendant ligand to synthesize a new copper(I) halide complex. We report here the crystal structure of $[\text{Cu}_2\text{Br}_2(\text{bppy})_2]_n$ (I).




Figure 1

View of the local coordination of Cu^{I} atoms, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. Atoms with the suffix A are generated by the symmetry code $(x, 1 + y, z)$.


Figure 2

The stair-like structure of (I). H atoms have been omitted for clarity.

tetrahedral coordination provided by three Br atoms and one N atom from bppy. Each Br atom bridges three copper atoms (Fig. 1), forming a zigzag stair-like structure along the b axis, as shown in Fig. 2.

In the crystal structure of (I), there are no supramolecular interactions, such as hydrogen bonds or π - π stacking forces.

Experimental

Compound (I) was hydrothermally synthesized under autogenous pressure. A mixture of bppy, CuSO_4 and water in a 2.1:5000 molar ratio was sealed in a Teflon-lined autoclave and heated at 453 K for 3 d. Red-orange needle-shaped crystals were obtained in about 42% yield.

Crystal data

$[\text{Cu}_2\text{Br}_2(\text{C}_{16}\text{H}_{11}\text{BrN}_2)_2]$	$D_x = 2.015 \text{ Mg m}^{-3}$
$M_r = 909.26$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 576 reflections
$a = 24.7379 (15) \text{ \AA}$	$\theta = 1.3\text{--}26.1^\circ$
$b = 3.9383 (2) \text{ \AA}$	$\mu = 6.78 \text{ mm}^{-1}$
$c = 32.063 (2) \text{ \AA}$	$T = 292 (2) \text{ K}$
$\beta = 106.3440 (10)^\circ$	Needle, red-orange
$V = 2997.5 (3) \text{ \AA}^3$	$0.40 \times 0.07 \times 0.05 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	5848 independent reflections
φ and ω scans	3560 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$R_{\text{int}} = 0.151$
$T_{\text{min}} = 0.554, T_{\text{max}} = 0.708$	$\theta_{\text{max}} = 26.1^\circ$
15498 measured reflections	$h = -27 \rightarrow 30$
	$k = -4 \rightarrow 4$
	$l = -39 \rightarrow 35$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.079$
 $wR(F^2) = 0.213$
 $S = 0.95$
 5848 reflections
 379 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.1201P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 1.34 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -2.40 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters ($\text{\AA}, ^\circ$).

N1—Cu1	2.013 (5)	Cu1—Br3 ⁱ	2.5523 (12)
N2—Cu2	2.026 (6)	Cu2—Br4	2.4291 (12)
Cu1—Br3	2.4615 (12)	Cu2—Br3 ⁱ	2.5518 (12)
Cu1—Br4	2.5262 (12)	Cu2—Br4 ⁱ	2.5584 (13)
N1—Cu1—Br3	119.79 (18)	N1—Cu1—Cu2	121.01 (18)
N1—Cu1—Br4	108.66 (17)	N2—Cu2—Br4	119.91 (18)
Br3—Cu1—Br4	110.02 (4)	N2—Cu2—Br3 ⁱ	105.64 (17)
N1—Cu1—Br3 ⁱ	104.30 (18)	Br4—Cu2—Br3 ⁱ	113.31 (4)
Br3—Cu1—Br3 ⁱ	103.52 (4)	N2—Cu2—Br4 ⁱ	106.57 (17)
Br4—Cu1—Br3 ⁱ	110.06 (4)	Br3 ⁱ —Cu2—Br4 ⁱ	106.19 (4)

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

All H atoms on C atoms were positioned geometrically and refined as riding, with $\text{C—H} = 0.93 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The high R_{int} value of 0.151 is the result of weak high-angle data. The highest peak is located 1.06 \AA from atom Br3 and the deepest hole 1.04 \AA from Br4.

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); software used to prepare material for publication: SHELXTL.

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