

**catena-Poly[[[bromocopper(I)]- $\mu$ -1,4-bis(imidazol-1-ylmethyl)benzene- $\kappa^2N^3:N^{3'}$ ] monohydrate]**

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**Key indicators**

Single-crystal X-ray study  
 T = 293 K  
 Mean  $\sigma(C-C)$  = 0.006 Å  
 H-atom completeness 88%  
 R factor = 0.046  
 wR factor = 0.143  
 Data-to-parameter ratio = 18.7

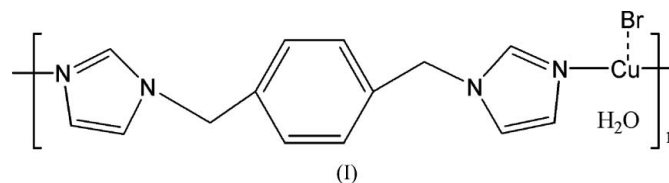
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound,  $[Cu(bix)Br]_n \cdot nH_2O$  [bix = 1,4-bis(imidazol-1-ylmethyl)benzene] or  $\{[CuBr(C_{14}H_{14}N_4)] \cdot H_2O\}_n$ , was synthesized by the hydrothermal method. The  $Cu^I$  centre has an unusual 2+1 trigonal coordination geometry. There is a crystallographic centre of inversion at the middle of each benzene ring. Each bix ligand binds with two  $Cu^I$  atoms to form a linear chain. These chains stack, forming micro-channels along the *a*-axis direction which are occupied by solvent water molecules.

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**Comment**

Recently, numerous studies have been concerned with the crystal engineering of metal-organic coordination polymers (Amabilino & Stoddart, 1995; Moulton & Zaworotko, 2001; Uppadine & Lehn, 2004). The synthetic strategies used to prepare these coordination polymers were mostly conventional solution methods using organic solvents. However, hydrothermal synthesis under pressure and at temperatures of 373–473 K proved to be an effective method. A variety of synthetic pathways were tested and completed successfully; these include oxidation, reduction and substitution reactions designed for preparing metal-organic coordination polymers (Chesnut *et al.*, 1999; Lu & Babb, 2002). Here, we have used the bix ligand [bix = 1,4-bis(imidazol-1-ylmethyl)benzene], 4,4'-bipyridine and  $Cu^{II}$  bromide to obtain a new polymer,  $[Cu(bix)Br]_n \cdot nH_2O$ , (I), under hydrothermal conditions. During the formation of (I), both reduction of  $Cu^{2+}$  and polymerization have occurred; reduction may be facilitated by the excess of N-donors during the reaction.



As shown in Fig. 1, the coordination environment of the  $Cu^I$  atom is trigonal planar. There is a crystallographic centre of inversion at the middle of the benzene ring of the bix ligand. The two coordinating N atoms from the bix ligands are oriented in a slightly bent arrangement with the  $Cu^I$  atom, and the Br atom forms a long semicoordinated  $Cu-Br$  bond (see Table 1 for selected bond lengths and angles). The weak  $Cu-Br$  interaction distorts the otherwise linear  $Cu1$  coordination towards trigonal geometry, resulting in an unusual 2+1 trigonal coordination geometry. The bridging bix ligands adopt a *trans* configuration, and the dihedral angles between planes  $N1/C1/$

N2/C3/C2 and C5/C6/C7A/C5A/C6A/C7, and N3/C8/N4/C9/C10 and C12/C13/C14B/C12B/C13B/C14 [symmetry codes: (A)  $1 - x, 2 - y, -z$ ; (B)  $2 - x, -y, 2 - z$ ] are  $76.2(2)$  and  $89.7(3)^\circ$ , respectively.

In the crystal structure of (I), two symmetry-related Cu<sup>I</sup> atoms are bridged by a bix ligand, forming a one-dimensional linear chain with Cu...Cu separations of  $14.258(3)$  and  $15.016(3)$  Å. In addition, the one-dimensional chains pack to form microchannels along the *a*-axis direction in which solvent water molecules are located (Fig. 2).

## Experimental

Bix dihydrate was prepared as described by Hoskins *et al.* (1997). Compound (I) was hydrothermally synthesized under autogenous pressure. A mixture of CuBr<sub>2</sub> (44.67 mg, 0.2 mmol), bix dihydrate (56 mg, 0.2 mmol), 4,4'-bipyridine (32 mg, 0.2 mmol) and H<sub>2</sub>O (8 ml) was sealed in a stainless reactor with a Teflon liner, which was heated to 453 K for 2 d. After slow cooling to room temperature, white block-shaped crystals of (I) were obtained as the major phase by filtration; these were washed with distilled water and finally dried in air.

### Crystal data

[CuBr(C <sub>14</sub> H <sub>16</sub> N <sub>4</sub> )]·H <sub>2</sub> O	$V = 784.6(4)$ Å <sup>3</sup>
$M_r = 399.76$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.692$ Mg m <sup>-3</sup>
$a = 8.855(2)$ Å	Mo $K\alpha$ radiation
$b = 9.723(3)$ Å	$\mu = 3.94$ mm <sup>-1</sup>
$c = 10.427(3)$ Å	$T = 293(2)$ K
$\alpha = 84.179(10)^\circ$	Block, white
$\beta = 75.926(10)^\circ$	$0.28 \times 0.12 \times 0.10$ mm
$\gamma = 64.305(8)^\circ$	

### Data collection

Rigaku Mercury 70 diffractometer	6268 measured reflections
$\omega$ scans	3562 independent reflections
Absorption correction: multi-scan ( <i>CrystalClear</i> ; Rigaku, 2000)	2314 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.841$ , $T_{\max} = 1.000$ (expected range = 0.567–0.674)	$R_{\text{int}} = 0.022$
	$\theta_{\text{max}} = 27.5^\circ$

### Refinement

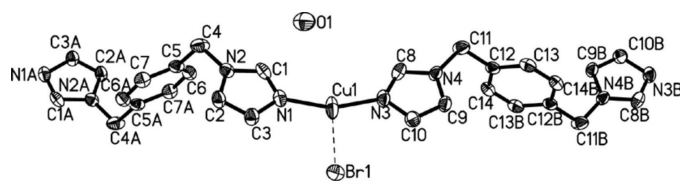
Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.046$	$w = 1/[\sigma^2(F_o^2) + (0.0779P)^2]$
$wR(F^2) = 0.143$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta\sigma)_{\text{max}} = 0.001$
3562 reflections	$\Delta\rho_{\text{max}} = 1.32$ e Å <sup>-3</sup>
190 parameters	$\Delta\rho_{\text{min}} = -1.01$ e Å <sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

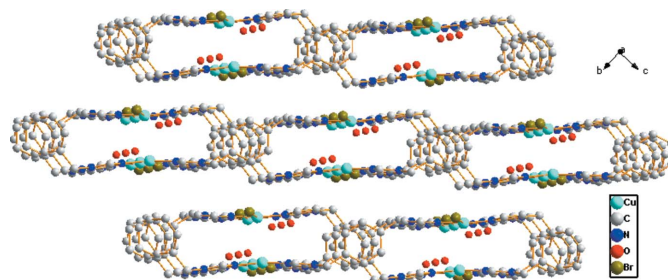
Cu1—N1	1.889(3)	Cu1—Br1	2.951(1)
Cu1—N3	1.884(3)		
N1—Cu1—N3	158.55(17)	C1—N1—Cu1	126.2(3)
N1—Cu1—Br1	99.66(11)	C3—N1—Cu1	127.8(3)
N3—Cu1—Br1	99.77(12)		

All H atoms bonded to carbon were placed in calculated positions, (C—H = 0.93–0.97 Å) and refined in the riding-model approximation



**Figure 1**

Part of the one-dimensional chain of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (A)  $1 - x, 2 - y, -z$ ; (B)  $2 - x, -y, 2 - z$ .]



**Figure 2**

The crystal structure of (I), showing the microchannels occupied by solvent water molecules. H atoms have been omitted.

with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The H atoms of the solvent water molecules could not be located and were not included in the refinement. The highest electron-density peak is  $0.97$  Å from atom Cu1 and the deepest hole is  $0.86$  Å from atom Cu1.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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