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***catena*-Poly[[[bis(perchlorato-*O*)-(1,10-phenanthroline-*N,N'*)-copper(II)]- $\mu$ -4,4'-bi-pyridine-*N:N'*] monohydrate]**

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**catena-Poly[[[bis(perchlorato-O)-  
(1,10-phenanthroline-*N,N'*)-  
copper(II)]- $\mu$ -4,4'-bipyridine-*N:N'*]  
monohydrate]**

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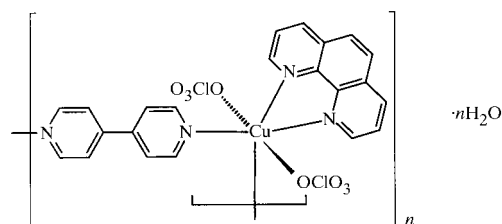
Data validation number: IUC0000213

The Cu atom in the title complex  $\{[\text{Cu}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{C}_{12}\text{H}_8\text{N}_2)(\text{ClO}_4)_2] \cdot \text{H}_2\text{O}\}_n$ , has an  $\text{N}_4\text{O}_2$  octahedral coordination geometry, the Cu atoms being bridged by the bipyridine and chelated by the phenanthroline heterocycles. Adjacent molecules are linked into a zigzag chain running along the *c* axis of the monoclinic unit cell. The chains are connected through lattice water molecules to produce a layer structure.

**Comment**

Coordination polymers that are constructed using 4,4'-bipyridine as the spacer exhibit a variety of topological motifs (Batten & Robson, 1998). Of particular interest are the motifs having cavities because small molecules can be clathrated (Fujita *et al.*, 1994; Janiak, 1997; Yaghi *et al.*, 1998; Kitagawa & Kondo, 1998; Hagrman *et al.*, 1999). We have reported a number of one-, two- and three-dimensional coordination polymers of 4,4'-bipyridine (abbreviated as 4,4'-bpy) and other related spacers (Chen *et al.*, 1996; Tong, Chen, Yu & Mak, 1998; Tong, Ye *et al.*, 1998; Tong, Chen, Ye & Ng, 1998; Tong, Zheng & Chen, 1999; Tong, Chen *et al.*, 1999; Tong, Lee *et al.*, 1999; Tong & Chen, 2000; Tong, Chen & Chen, 2000). Our attempt to obtain a two-dimensional architecture with copper perchlorate that is chelated by 1,10-phenanthroline (phen) gave only one-dimensional  $[\text{Cu}(4,4'\text{-bpy})(\text{phen})(\text{ClO}_4)_2] \cdot \text{H}_2\text{O}$ , (I).

The Cu atom shows octahedral coordination. Two N atoms from a pair of *cis*-related 4,4'-bpy ligands coordinate to the Cu atom [Cu–N 2.009 (4) and 2.025 (5) Å], which is chelated by the phen heterocycle [Cu–N 1.998 (4) and 2.028 (5) Å]. The perchlorate anions are *trans* to each other, but one is much farther from the Cu atom than the other [Cu–O 2.377 (5) and 2.728 (5) Å]. The Cu–N<sub>phen</sub> distances are similar to those found in other phen complexes (Baggio *et al.*, 1995; Solans *et al.*, 1990) and the Cu–N(4,4'-bpy) distances are also similar to



(I)

those found in related complexes (Chen *et al.*, 1992, 1996; Tong, Chen, Yu & Mak, 1998; Tong, Ye *et al.*, 1998; Tong & Chen, 2000; Tong, Chen & Chen, 2000).

In the zigzag  $[\text{Cu}(4,4'\text{-bpy})(\text{phen})(\text{ClO}_4)_2]_n$  chains, the metal atoms are 10.93 Å apart. The separation is also observed in *catena*-(2,2'-bpy)(ClO<sub>4</sub>)( $\mu$ -2-4,4'-bpy)Cu (Chen *et al.*, 1992) and *catena*-( $\mu$ -2-4,4'-bpy)(CH<sub>3</sub>N)<sub>2</sub>(2,9-dimethylphen)Cu<sup>I</sup>·BF<sub>4</sub> (Blake *et al.*, 1998). However, the rings of the 4,4'-bpy bridge are twisted by 41.4 (1)°, whereas those in (2,2'-bpy)(ClO<sub>4</sub>)( $\mu$ -2-4,4'-bpy)Cu are coplanar (Chen *et al.*, 1992).

In (I), the lattice water molecule forms hydrogen bonds to perchlorate of two adjacent chains [O...O = 2.64 (2) and 3.00 (2) Å], that to the strongly bonded perchlorate being much longer than that to weakly bonded ion.

**Experimental**

Phen (1 mmol) dissolved in a small volume of ethanol (4 ml) was added to Cu(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O (1 mmol) dissolved in water (10 ml). To the warm solution was added 4,4'-bpy (1 mmol) dissolved in ethanol (5 ml), followed by NaClO<sub>4</sub> (2 mmol) in water (5 ml). Crystals precipitated from solution after a few days in almost quantitative yield.

*Crystal data*

$[\text{Cu}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{C}_{12}\text{H}_8\text{N}_2)(\text{ClO}_4)_2] \cdot \text{H}_2\text{O}$   
*M<sub>r</sub>* = 616.84  
Monoclinic, *P*2<sub>1</sub>/*n*  
*a* = 12.553 (1) Å  
*b* = 14.4169 (9) Å  
*c* = 13.2205 (9) Å  
 $\beta$  = 94.377 (7)°  
*V* = 2385.5 (3) Å<sup>3</sup>  
*Z* = 4

*D<sub>x</sub>* = 1.717 Mg m<sup>-3</sup>  
Mo *K*α radiation  
Cell parameters from 25 reflections  
 $\theta$  = 7.5–15°  
 $\mu$  = 1.202 mm<sup>-1</sup>  
*T* = 298 (2) K  
Block, blue  
0.42 × 0.36 × 0.34 mm

*Data collection*

Siemens *R3m* diffractometer  
 $\omega$  scans  
Absorption correction:  $\psi$  scan (North *et al.*, 1968)  
*T<sub>min</sub>* = 0.596, *T<sub>max</sub>* = 0.665  
5775 measured reflections  
4185 independent reflections  
2883 reflections with *I* > 2σ(*I*)

*R<sub>int</sub>* = 0.004  
 $\theta_{\text{max}}$  = 24.98°  
*h* = 0 → 14  
*k* = 0 → 17  
*l* = -15 → 15  
2 standard reflections every 120 reflections  
intensity decay: none

*Refinement*

Refinement on *F*<sup>2</sup>  
 $R[F^2 > 2\sigma(F^2)]$  = 0.061  
*wR(F<sup>2</sup>)* = 0.173  
*S* = 1.028  
4187 reflections  
343 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0826P)^2 + 6.1274P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.61 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.77 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

Cu1—N1	1.998 (4)	Cu1—N4 <sup>i</sup>	2.025 (5)
Cu1—N2	2.028 (5)	Cu1—O1	2.382 (4)
Cu1—N3	2.009 (4)	Cu1—O5	2.731 (5)
N1—Cu1—N2	82.0 (2)	N2—Cu1—O5	89.8 (2)
N1—Cu1—N3	169.7 (2)	N3—Cu1—N4 <sup>i</sup>	87.9 (2)
N1—Cu1—N4 <sup>i</sup>	96.2 (2)	N3—Cu1—O1	92.7 (2)
N1—Cu1—O1	96.5 (2)	N3—Cu1—O5	92.2 (2)
N1—Cu1—O5	78.6 (2)	N4 <sup>i</sup> —Cu1—O1	93.7 (2)
N2—Cu1—N3	93.5 (2)	N4 <sup>i</sup> —Cu1—O5	87.5 (2)
N2—Cu1—N4 <sup>i</sup>	177.0 (2)	O1—Cu1—O5	175.1 (2)
N2—Cu1—O1	88.9 (2)		

Symmetry codes: (i)  $\frac{1}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$ .

**Table 2**

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1W—H1W1...O4	0.90	2.13	3.00 (2)	159
O1W—H1W2...O8 <sup>i</sup>	0.90	2.22	2.64 (2)	108

Symmetry codes: (i)  $x - \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} + z$ .

The Cl—O distances in the anions were restrained to be approximately equal. C-bonded H atoms were treated as riding (C—H = 0.93 Å). The water H atoms were placed at calculated positions.

Data collection: *R3m Software* (Siemens, 1990); cell refinement: *R3m Software*; data reduction: *R3m Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); software used to prepare material for publication: *SHELXL97*.

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