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#### Key indicators

Single-crystal X-ray study

$T = 293\text{ K}$

Mean  $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$

Disorder in solvent or counterion

$R$  factor = 0.053

$wR$  factor = 0.169

Data-to-parameter ratio = 12.2

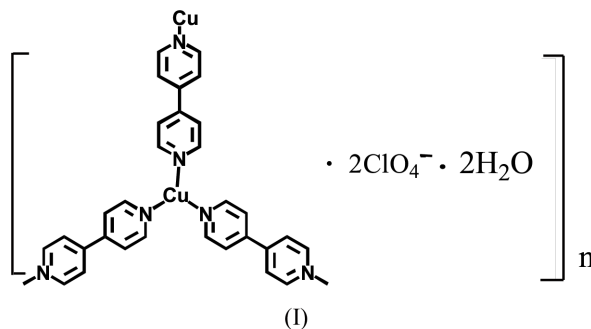
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## Poly[[dicopper(I)-tri- $\mu$ -4,4'-bipyridyl] diperchlorate dihydrate]

The title compound,  $\{[\text{Cu}_2(\text{C}_{10}\text{H}_8\text{N}_2)_3](\text{ClO}_4)_2 \cdot 2\text{H}_2\text{O}\}_n$ , forms a three-dimensional network containing one-dimensional nanoporous channels, accommodating guest water molecules and perchlorate anions. The network consists of  $[\text{Cu}_2(4,4'\text{-bipyridyl})_3]^{2+}$  cations containing trigonal planar  $\text{Cu}^{\text{I}}$  centers bonded to three 4,4'-bipyridyl groups.

#### Comment

The crystal engineering of microporous polymers is currently of great interest, owing to their intriguing topologies and potential applications in gas adsorption or storage, ion-exchange, heterogeneous catalysis and so on (Dyer, 1988). The linear bifunctional ligand 4,4'-bipyridyl has been applied widely for the construction of microporous materials (Yaghi & Li, 1995; Noro *et al.*, 2002; Inman *et al.*, 2002). In this paper, we report a new three-dimensional coordination polymer,  $\{[\text{Cu}_2(4,4'\text{-bipyridyl})_3](\text{ClO}_4)_2 \cdot 2\text{H}_2\text{O}\}_n$  (I).



The asymmetric unit of (I) consists of one-half of a  $[\text{Cu}_2(4,4'\text{-bipyridyl})_3]^{2+}$  cation, one-half of each of two  $\text{ClO}_4^-$  anions and a water molecule (Fig. 1). The other half of the cation is generated by the symmetry operations  $(x, \frac{1}{4} - y, \frac{1}{4} - z)$  and  $(x - \frac{1}{4}, 1 - y, z - \frac{1}{4})$ , whereas the other halves of the anions are generated by the symmetry operations  $(\frac{3}{4} - x, \frac{3}{4} - y, z)$  and  $(x, \frac{1}{4} - y, \frac{1}{4} - z)$ , respectively. The  $\text{Cu}^{\text{I}}$  atom shows a slightly distorted trigonal planar arrangement.

The structure determination shows that the symmetry-equivalent cations are linked to form interpenetrating three-dimensional networks similar to those observed in  $\text{Cu}(4,4'\text{-bipyridyl})_{1.5} \cdot \text{NO}_3 \cdot 1.5\text{H}_2\text{O}$  (Yaghi & Li, 1995). The only differences between the two compounds are the guest anions and the number of water molecules.

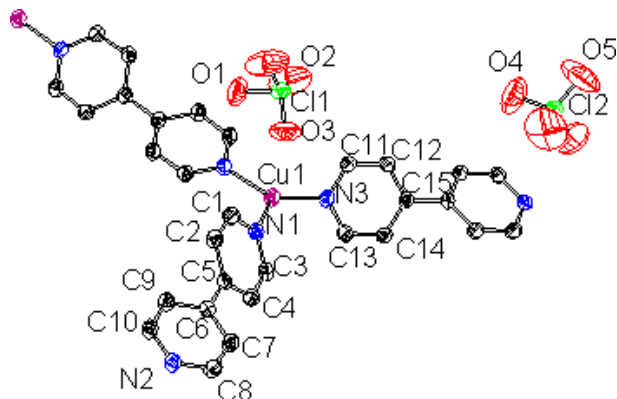
#### Experimental

A mixture of  $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$  (0.186 g, 0.5 mmol), 4,4'-bipyridyl (0.091 g, 0.3 mmol), acetylenedicarboxylic acid (0.057 g, 0.5 mmol) and water (10 ml) was sealed in a 15 ml Teflon-lined stainless-steel

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**Figure 1**

The molecular structure of (I), showing 20% probability displacement ellipsoids. The atom-numbering scheme is shown only for the contents of the asymmetric unit, and H atoms have been omitted for clarity. Atom O1 is disordered over two positions, each with an occupancy of 0.50.

reactor and heated to 433 K for 60 h, yielding yellow crystals of (I) suitable for X-ray analysis.

**Crystal data**

$[\text{Cu}_2(\text{C}_{10}\text{H}_8\text{N}_2)_3](\text{ClO}_4)_2 \cdot 2\text{H}_2\text{O}$   
 $M_r = 830.56$   
 Orthorhombic, *Fddd*  
 $a = 18.7770$  (8) Å  
 $b = 23.3593$  (13) Å  
 $c = 30.4231$  (16) Å  
 $V = 13344.1$  (12) Å<sup>3</sup>  
 $Z = 16$   
 $D_x = 1.654$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
 Cell parameters from 200 reflections  
 $\theta = 1.5\text{--}25.0^\circ$   
 $\mu = 1.50$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Prism, yellow  
 $0.56 \times 0.40 \times 0.22$  mm

**Data collection**

Siemens SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  
 $T_{\min} = 0.538$ ,  $T_{\max} = 0.719$   
 7804 measured reflections

2938 independent reflections  
 2014 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.038$   
 $\theta_{\text{max}} = 25.0^\circ$   
 $h = -22 \rightarrow 12$   
 $k = -19 \rightarrow 27$   
 $l = -35 \rightarrow 35$

**Refinement**

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.053$   
 $wR(F^2) = 0.169$   
 $S = 1.00$   
 2938 reflections  
 241 parameters  
 H-atoms treated by a mixture of independent and constrained refinement

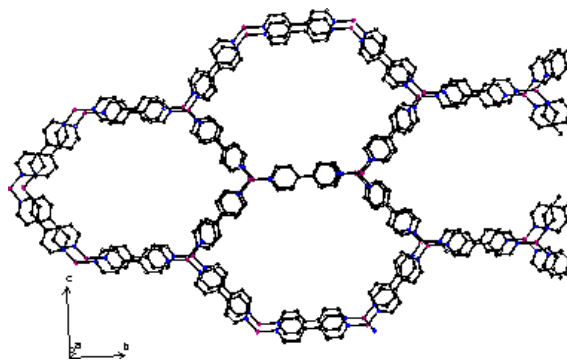
$w = 1/[\sigma^2(F_o^2) + (0.089P)^2 + 84.2861P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.004$   
 $\Delta\rho_{\text{max}} = 0.62$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.36$  e Å<sup>-3</sup>  
 Extinction correction: *SHELXTL*  
 Extinction coefficient: 0.00015 (3)

**Table 1**

Selected geometric parameters (Å, °).

Cu1—N3	1.962 (4)	Cu1—N1	2.003 (4)
Cu1—N2 <sup>i</sup>	1.999 (4)		
N3—Cu1—N2 <sup>i</sup>	125.03 (17)	N2 <sup>i</sup> —Cu1—N1	111.21 (17)
N3—Cu1—N1	123.65 (17)		

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

**Figure 2**

A view, down the *a* axis, of the cationic framework.

**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—H1WB···O1	0.81 (8)	1.97 (9)	2.771 (14)	168 (9)
O1W—H1WA···O5 <sup>ii</sup>	0.74 (8)	2.17 (8)	2.877 (13)	159 (9)

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

H atoms bonded to C atoms were placed at calculated positions ( $\text{C—H} = 0.93$  Å) and refined using a riding model, with isotropic displacement parameters set to  $1.2U_{\text{eq}}(\text{C})$ . H atoms of the water molecule were located in a difference map and refined freely. Atom O1 is disordered over two positions, each with an occupancy of 0.50.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART* and *SAINT* (Siemens, 1994); data reduction: *SAINT* and *XPREP* in *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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