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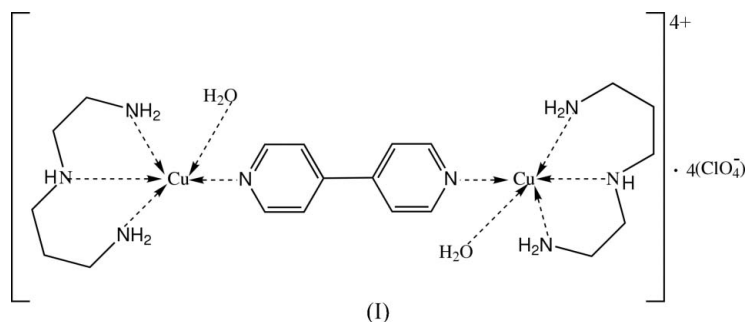
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## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.009$  Å  
Disorder in solvent or counterion  
 $R$  factor = 0.061  
 $wR$  factor = 0.160  
Data-to-parameter ratio = 11.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>. **$\mu$ -4,4'-Bipyridine- $\kappa^2\text{N}:\text{N}'$ -bis{[ $N$ -(2-aminoethyl)-1,3-propyldiamine- $\kappa^3\text{N},\text{N}',\text{N}''$ ]} aqua-copper(II)} tetrakis(perchlorate)**The title dinuclear copper complex,  $[\{\text{Cu}(\text{C}_5\text{H}_{15}\text{N}_3)(\text{H}_2\text{O})\}_2(\text{C}_{10}\text{H}_8\text{N}_2)](\text{ClO}_4)_4$ , has a crystallographically imposed inversion centre. Each  $\text{Cu}^{\text{II}}$  atom is coordinated by four N atoms [ $\text{Cu}-\text{N} = 2.001(4)$ – $2.037(4)$  Å] and one water molecule [ $\text{Cu}-\text{O} = 2.373(3)$  Å] in a slightly distorted square-pyramidal geometry.

## Comment

The linear bidentate ligand 4,4'-bipyridine is widely used as a building block in designing coordination polymers, which possess potentially useful physical, chemical and biological properties (Wainwright, 1997). Here we present the crystal structure of the title dinuclear complex, (I), in which two Cu atoms are bridged by the 4,4'-bipyridine ligand.

In (I), each  $\text{Cu}^{\text{II}}$  atom is coordinated by four N atoms and one water molecule (Fig. 1) in a slightly distorted square-pyramidal geometry (Table 1). The value of the  $\tau$  parameter (0.06) indicates an almost ideal square-pyramidal shape of the coordination polyhedron (Addison *et al.*, 1984). Atoms N1, N2, N3 and N4 define the basal plane, whereas the apical position is occupied by water atom O1. The average deviation of the four N atoms from the basal plane is 0.034 Å, while the Cu1 atom is displaced by 0.143(3) Å from this plane toward the apex. The dinuclear cation is centrosymmetric.The perchlorate anions are involved in the formation of intermolecular  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 2), which stabilize the crystal structure (Fig. 2).

## Experimental

To a stirred solution of  $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$  (1 mmol) and  $N$ -(2-aminoethyl)propane-1,3-diamine (1 mmol) in absolute methanol (15 ml), a methanol solution (15 ml) of 4,4'-bipyridine (0.5 mmol) was added at room temperature. After stirring for 2 h at 320 K, the precipitate was filtered off, washed with methanol and dried *in vacuo*. Blue single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of the filtrate at ambient temperature after 10 d.

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## Crystal data

[Cu<sub>2</sub>(C<sub>10</sub>H<sub>21</sub>N<sub>4</sub>O)<sub>2</sub>](ClO<sub>4</sub>)<sub>4</sub> $M_r = 951.50$ Monoclinic,  $P2_1/n$  $a = 7.6572$  (9) Å $b = 17.218$  (2) Å $c = 14.4430$  (17) Å $\beta = 98.359$  (2)° $V = 1884.0$  (4) Å<sup>3</sup> $Z = 2$  $D_x = 1.677$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation $\mu = 1.49$  mm<sup>-1</sup> $T = 293$  (2) K

Block, blue

 $0.34 \times 0.30 \times 0.28$  mm

## Data collection

Bruker APEX area-detector diffractometer

 $\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2002)

 $T_{\min} = 0.631$ ,  $T_{\max} = 0.680$ 

13315 measured reflections

3311 independent reflections

2755 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.027$  $\theta_{\text{max}} = 25.0^\circ$ 

## Refinement

Refinement on  $F^2$  $R[F^2 > 2\sigma(F^2)] = 0.061$  $wR(F^2) = 0.160$  $S = 1.07$ 

3311 reflections

300 parameters

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0813P)^2 + 2.7723P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\text{max}} < 0.001$  $\Delta\rho_{\text{max}} = 0.78$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.42$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Cu1—N4	2.000 (5)	Cu1—N1	2.038 (4)
Cu1—N2	2.006 (4)	Cu1—O1	2.372 (4)
Cu1—N3	2.037 (4)		
N4—Cu1—N2	173.2 (2)	N3—Cu1—N1	169.45 (19)
N4—Cu1—N3	84.06 (19)	N4—Cu1—O1	92.60 (19)
N2—Cu1—N3	92.54 (19)	N2—Cu1—O1	93.58 (18)
N4—Cu1—N1	91.76 (18)	N3—Cu1—O1	95.69 (18)
N2—Cu1—N1	90.58 (18)	N1—Cu1—O1	94.17 (16)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2A $\cdots$ O7 <sup>i</sup>	0.90	2.05	2.880 (14)	154
N2—H2A $\cdots$ O7 <sup>i</sup>	0.90	2.44	3.336 (10)	172
N2—H2B $\cdots$ O9 <sup>i</sup>	0.90	2.36	3.17 (2)	150
N2—H2B $\cdots$ O8	0.90	2.43	3.280 (12)	158
N3—H3 $\cdots$ O8 <sup>i</sup>	0.91	2.30	2.972 (19)	131
N3—H3 $\cdots$ O6	0.91	2.46	3.337 (10)	162
N4—H4A $\cdots$ O2 <sup>ii</sup>	0.90	2.43	3.078 (7)	129
N4—H4A $\cdots$ O4 <sup>ii</sup>	0.90	2.49	3.292 (14)	149
N4—H4A $\cdots$ O4 <sup>ii</sup>	0.90	2.52	3.408 (16)	169
N4—H4B $\cdots$ O7 <sup>iii</sup>	0.90	2.26	3.067 (9)	149
N4—H4B $\cdots$ O7 <sup>iii</sup>	0.90	2.35	3.202 (18)	157
O1—H1A $\cdots$ O5 <sup>iv</sup>	0.85	2.05	2.886 (16)	168
O1—H1A $\cdots$ O3 <sup>iv</sup>	0.85	2.46	2.991 (17)	122
O1—H1A $\cdots$ O5 <sup>iv</sup>	0.85	2.46	3.31 (2)	171
O1—H1B $\cdots$ O6 <sup>iii</sup>	0.85	2.10	2.832 (17)	144
O1—H1B $\cdots$ O8 <sup>iii</sup>	0.85	2.33	3.169 (13)	172

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

H atoms were positioned geometrically ( $C-H = 0.93-0.97$  Å,  $N-H = 0.90$  Å and  $O-H = 0.85$  Å) and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$ . The two crystallographically independent perchlorate anions were treated as rotationally disordered over two

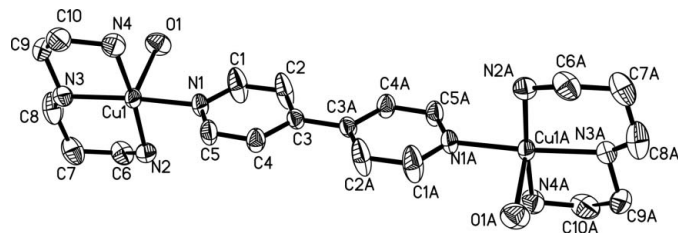


Figure 1

The molecular structure of the title complex, showing the atomic labelling and displacement ellipsoids drawn at the 30% probability level [symmetry code: (A)  $-x, 1-y, 1-z$ ]. The perchlorate anions and H atoms have been omitted for clarity.

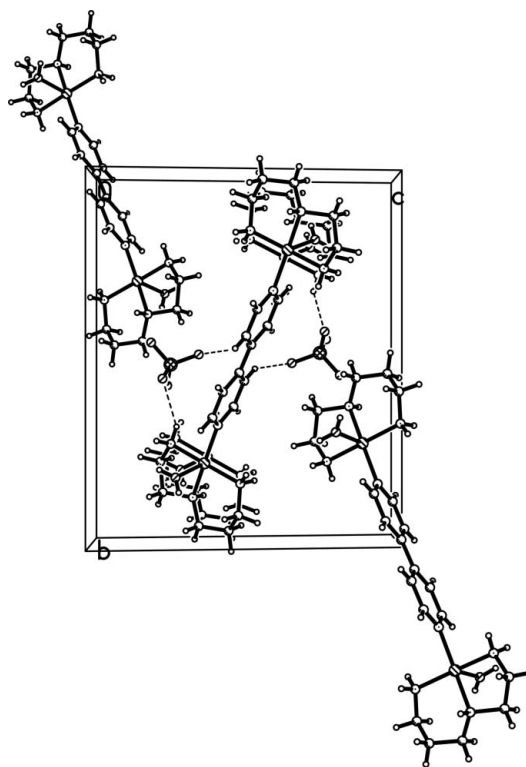


Figure 2

A portion of the crystal packing, viewed down the  $a$  axis, showing the intermolecular hydrogen bonds as dashed lines. Only the major components of the disordered perchlorate anions are shown.

orientations each, with refined occupancies of 0.512 (19) and 0.488 (19) for the first anion, and 0.672 (8) and 0.328 (8) for the second anion.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINTE* (Bruker, 2003); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXLTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXLTL*.

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