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Poly[[dicopper(II)-μ-4,4′-bipyridyl-bis[μ-*N*-(hydroxypropyl)propane-1,3-diamine]] bis(perchlorate)]

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Key indicators

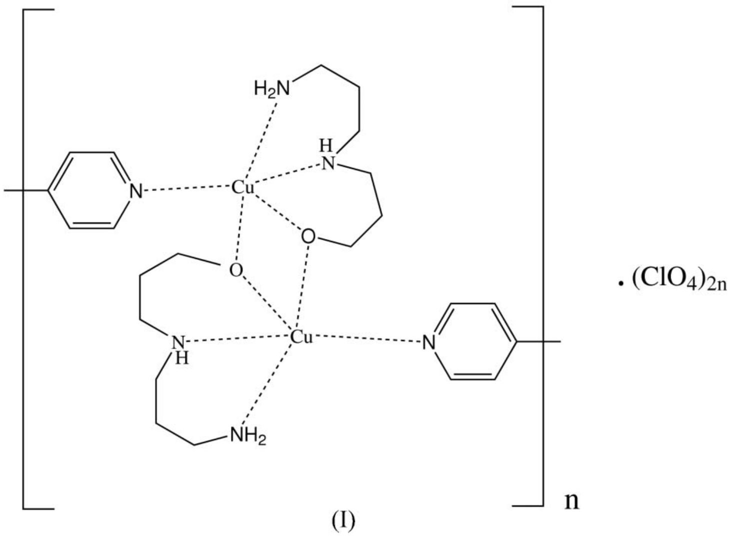
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.015 Å
Disorder in main residue
R factor = 0.066
wR factor = 0.210
Data-to-parameter ratio = 13.1

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

The title coordination polymer, $\{[Cu_2(C_6H_{15}N_2O)_2(C_{10}H_8N_2)](ClO_4)_2\}_n$, was synthesized from 4,4′-bipyridine, *N*-hydroxypropyl-1,3-propanediamine and copper(II) perchlorate. Structural analysis shows that each copper ion is coordinated by the 4,4′-bipyridine molecule through one N atom, and by two *N*-hydroxypropyl-1,3-propanediamine ligands through the O atom and two N atoms of one, and the O atom from the second, giving a distorted square-pyramidal geometry. There are centres of inversion at the mid-points of the Cu_2O_2 ring and the bridging ligand.

Comment

The construction and characterization of coordination polymers has increasingly become one of the most important fields in supramolecular chemistry, crystal engineering and materials science (Li *et al.*, 2006). The linear bidentate ligand 4,4′-bipyridine is widely used as a building block in designing coordination polymers that possess potentially useful physical, chemical and biological properties (Wainwright, 1997). Here we report the synthesis and structure of a new one-dimensional copper(II) coordination polymer obtained from the self-assembly of *N*-hydroxypropyl-1,3-propanediamine, 4,4′-bipyridine and Cu^{II} ions.



(I)

The title complex, (I), consists of copper(II) ions, 4,4′-bipyridine and *N*-hydroxypropyl-1,3-propanediamine ligands, with 4,4′-bipyridine acting as a centrosymmetric bridging ligand, forming a one-dimensional arrangement (Fig. 1). The five-coordinate N_3O_2 environment around the Cu^{II} atom is in the form of a slightly distorted square pyramid (Fig. 2), as

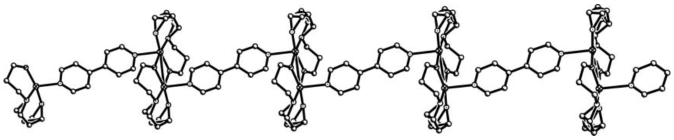


Figure 1
The one-dimensional chain structure of the title complex. H atoms and perchlorate ions have been omitted for clarity.

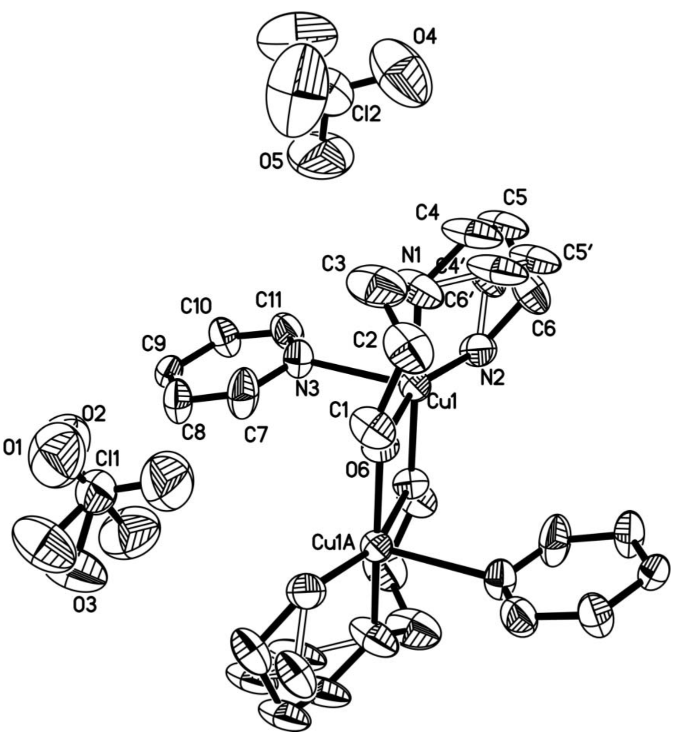


Figure 2
Part of the polymeric structure of the title compound, showing the disorder, atom-labelling scheme and displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry code: (A) $\frac{3}{2} - x, \frac{1}{2} - y, -z$].

indicated by the value of the τ parameter (0.21) (Addison *et al.*, 1984). The basal plane is formed by N1, N2, O6 and O6^{i} [symmetry code: (i) $\frac{3}{2} - x, \frac{1}{2} - y, -z$], while the apical position is occupied by atom N3 of the 4,4′-bipyridine ligand. The Cu1 ion is displaced by 0.119 (3) Å from this plane toward the apex, and N3 is displaced by 2.601 (8) Å from the basal plane. The Cu_2O_2 four-membered ring is centrosymmetric.

Atom N1 of the *N*-hydroxypropyl-1,3-propanediamine ligand forms an intramolecular hydrogen bond with atom N3, while N2 forms intermolecular hydrogen bonds with atoms O1 and O4 of two different perchlorate anions.

Experimental

To a stirred solution of $Cu(ClO_4)_2 \cdot 6H_2O$ (1 mmol) and *N*-hydroxypropyl-1,3-propanediamine (1 mmol) in absolute methanol (15 ml) was added a methanol solution (15 ml) of 4,4′-bipyridine (0.5 mmol) 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 analysis were obtained by slow evaporation of the filtrate at ambient temperature after 15 d.

Crystal data

$[Cu_2(C_6H_{15}N_2O)_2(C_{10}H_8N_2)](ClO_4)_2$
M_r = 744.56
Monoclinic, $C2/c$
a = 11.989 (2) Å
b = 19.699 (3) Å
c = 13.297 (3) Å
β = 91.175 (3)°
V = 3139.7 (10) Å^3
Z = 4
D_x = 1.575 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.58 mm^{-1}
T = 293 (2) K
Block, blue
0.40 × 0.32 × 0.28 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.570, T_{max} = 0.665
8102 measured reflections
2748 independent reflections
1223 reflections with $I > 2\sigma(I)$
R_{int} = 0.083
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.210
S = 1.00
2748 reflections
210 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.096P)^2 +]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—N1	1.973 (8)	Cu1—O6	1.923 (5)
Cu1—N2	1.996 (6)	Cu1—O6^{i}	2.444 (5)
Cu1—N3	2.411 (8)	Cu1···Cu1^{i}	3.0498 (19)

Symmetry code: (i) $-x + \frac{3}{2}, -y + \frac{1}{2}, -z$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N3	0.91	2.68	3.163 (12)	114
N2—H2A···O1^{ii}	0.90	2.32	3.173 (14)	159
N2—H2B···O4^{iii}	0.90	2.47	3.119 (13)	129

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

Bipyridine H atoms were placed in calculated positions, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). Methylene H atoms and amino H atoms were positioned geometrically, with C—H = 0.97 Å and N—H = 0.90 Å, and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C,N). The presence of disorder was identified from a difference Fourier map for C4, C5 and C6, and O2 and O3 of one of the perchlorate ions (which lies on a twofold rotation axis). Disordered atoms were refined by applying appropriate restraints to the bond lengths [1.53 (2) for C—C, 1.47 (2) for C—N, 1.40 (2) for Cl—O and 2.32 (2) Å for O···O] and displacement parameters. The site occupancies for C4, C5, C6 and C4′, C5′, C6′, were found to be 0.689 (16) and 0.311 (16), respectively; while for O2,O3 and O2′,O3′ they were fixed at 0.501 and 0.499, respectively, while for the perchlorate O atoms they are exactly 0.5 by symmetry.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics:

Acta Cryst. (2007). E**63**, m172–m174 Zhang *et al.* • $[Cu_2(C_6H_{15}N_2O)_2(C_{10}H_8N_2)](ClO_4)_2$ **m173**

SHELXTL (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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