The two-dimensional structure of poly[[diperchloratocopper(II)]-bis[μ_2-1,3-bis(4-pyridyl)propane]]

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.007 Å
R factor = 0.057
wR factor = 0.159
Data-to-parameter ratio = 14.0

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

In the crystal structure of the title compound, $[Cu(ClO_4)_2(C_{13}H_{14}N_2)_2]_n$, there are two independent Cu^{II} ions, one of which occupies a crystallographic inversion center. The 1,3-bis(4-pyridyl)propane ligands bridge the Cu^{II} ions to form two independent two-dimensional sheets. In addition, two terminal perchlorate anions are coordinated to each Cu^{II} ion, resulting in distorted octahedral coordination around each Cu^{II} ion. The equatorial Cu—N bonds are in the range 2.014 (4)–2.031 (4) Å, while the long axial Cu—O distances range from 2.434 (3) to 2.548 (3) Å.

Comment

Self-assembly processes involving metal ions and organic ligands directed by either metal coordination preferences or hydrogen bonds have attracted much attention in the fields of supramolecular and coordination chemistry (Barnett & Champness, 2003; Batten & Robson, 1998). Materials utilizing rigid or flexible spacer ligands have been studied because of their potential as building blocks for supramolecular assemblies, and their ability to act as optical sensors and heterogeneous catalysts (Balzani *et al.*, 1996; Hong *et al.*, 2004; Leininger *et al.*, 2000). In our attempt to investigate the design and control of the self-assembly of coordination polymers with flexible bridging ligands, we have employed copper perchlorate to prepare the title compound, (I), a new polymeric complex with the ligand 1,3-bis(4-pyridyl)propane.

(I)
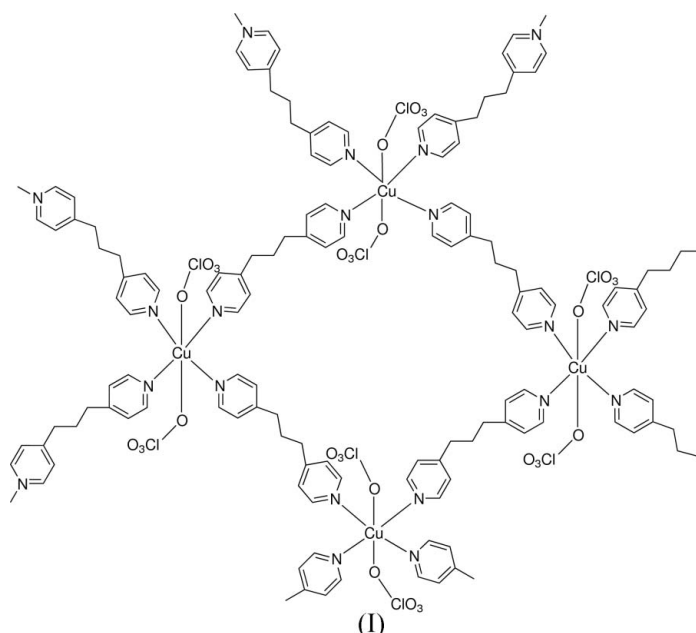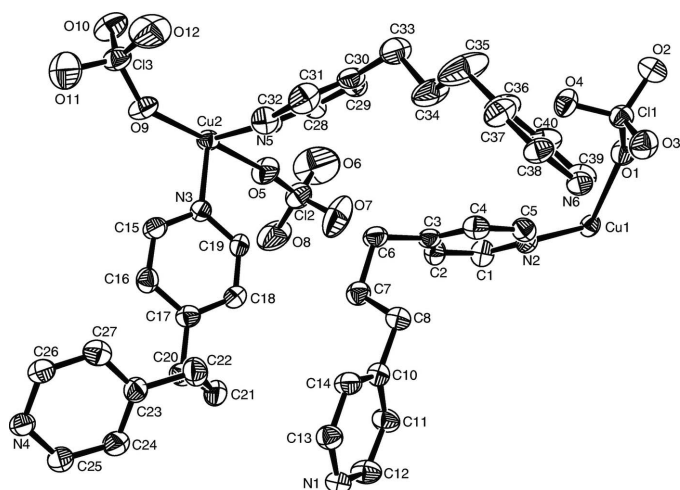
Figure 1
The asymmetric unit of (I), showing 50% probability displacement ellipsoids (H atoms omitted for clarity).

Figure 2
Structures of the two-dimensional sheets in (I). The red bonds represent a sheet containing Cu1, and the black bonds a sheet containing Cu2.

The asymmetric unit of (I) contains two different Cu coordination centers (Fig. 1), atom Cu1 being located on a crystallographic inversion center. The 1,3-bis(4-pyridyl)-propane ligands bridge the two different Cu^{II} ions to form two independent two-dimensional sheets (Fig. 2). For both types of Cu^{II} ion, the 1,3-bis(4-pyridyl)propane ligands coordinate through N atoms [Cu—N = 2.014 (4)–2.031 (4) Å] in the equatorial positions, while two perchlorate anions are coordinated to each Cu^{II} ion with long axial Cu—O bonds [2.434 (3)–2.548 (3) Å] to complete a distorted octahedral coordination. The 1,3-bis(4-pyridyl)propane ligand has been shown to adopt four different conformations (Carlucci *et al.*, 1997; Plater *et al.*, 2000). In (I), the ligand is in a *trans–cis* conformation for the sheet containing Cu1 (Fig. 3) and a *trans–trans* conformation for the sheet containing Cu2 (Fig. 4).

Experimental

Violet crystals of (I) appeared when an aqueous solution (10 ml) of $Cu(ClO_4)_2 \cdot 6H_2O$ (0.185 g, 0.5 mmol) was carefully layered with a methanol solution (10 ml) of 1,3-bis(4-pyridyl)propane (0.198 g, 1 mmol).

Crystal data

$[Cu(ClO_4)_2(C_{13}H_{14}N_2)_2]$	$D_x = 1.483$ Mg m^{-3}
$M_r = 658.96$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 27195
$a = 15.0179$ (5) Å	reflections
$b = 16.2881$ (5) Å	$\theta = 2.6$–27.5°
$c = 18.5719$ (7) Å	$\mu = 0.98$ mm^{-1}
$\beta = 102.9642$ (13)°	$T = 150$ (1) K
$V = 4427.2$ (3) Å^3	Block, violet
$Z = 6$	$0.10 \times 0.08 \times 0.06$ mm

Data collection

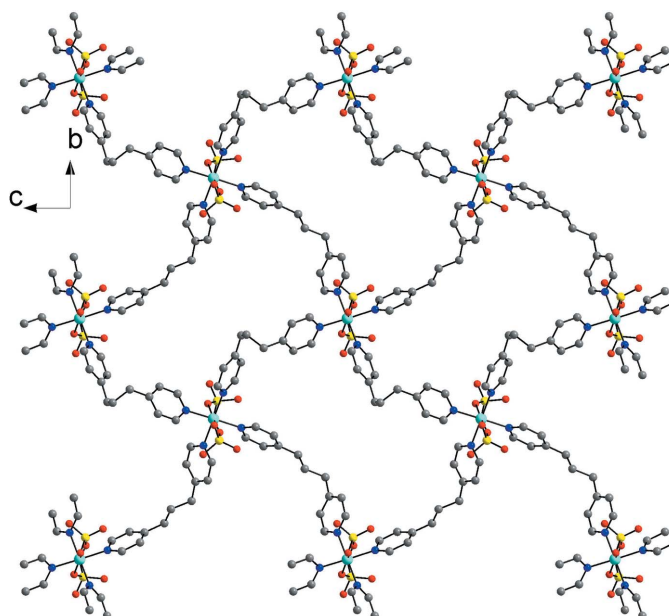|	
Bruker–Nonius KappaCCD	7778 independent reflections
diffractometer	5253 reflections with $I > 2\sigma(I)$
φ scans and ω scans with κ offsets	$R_{int} = 0.097$
Absorption correction: multi-scan	$\theta_{max} = 25.0°$
(*SORTAV*; Blessing, 1995)	$h = -17 \rightarrow 16$
$T_{min} = 0.689$, $T_{max} = 0.952$	$k = -18 \rightarrow 19$
27195 measured reflections	$l = -21 \rightarrow 22$

Figure 3
Two-dimensional sheet containing Cu1 atoms.

Figure 4
Two-dimensional sheet containing Cu2 atoms.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0775P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.057$	$+ 2.2199P]$
$wR(F^2) = 0.159$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
7778 reflections	$\Delta\rho_{max} = 0.46$ e Å^{-3}
557 parameters	$\Delta\rho_{min} = -0.68$ e Å^{-3}
H-atom parameters constrained	Extinction correction: *SHELXL97*
	Extinction coefficient: 0.0013 (3)

Table 1
Selected interatomic distances (Å).

Cu1—N1^i	2.014 (3)	Cu2—N6^{iii}	2.023 (3)
Cu1—N2	2.022 (4)	Cu2—N5	2.031 (4)
Cu1—O1	2.548 (3)	Cu2—O5	2.434 (3)
Cu2—N4^{ii}	2.014 (4)	Cu2—O9	2.447 (3)
Cu2—N3	2.014 (4)		

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

The displacement ellipsoids for atoms C34 and C35 suggest that they might be disordered over two positions, but this disorder was not resolved. H atoms were placed in calculated positions, with C—H distances of 0.95 Å (pyridyl) and 0.99 Å (methylene). They were included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}$(carrier).

Data collection: *COLLECT* (Nonius, 2003); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXTL/PC* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL/PC*; molecular graphics: *SHELXTL/PC*; software used to prepare material for publication: *SHELXTL/PC*.

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