

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

Ji Young Ryu,^a Cheal Kim,^{a*}
 Dae Won Park,^b Lae Ok Park,^c
 Youngmee Kim^{d*} and Alan J.
 Lough^e

^aDepartment of Fine Chemistry, Seoul National University of Technology, Seoul 139-743, South Korea, ^bDepartment of Energy and Environmental Engineering, Seoul National University of Technology, Seoul 139-743, South Korea, ^c646-9 BH Biomedic Company, Yeoksam-Dong, Kangnam-Gu, Seoul 135-911, South Korea, ^dDivision of Nano Sciences, Ewha Women's University, Seoul 120-750, South Korea, and ^eDepartment of Chemistry, University of Toronto, Ontario, Canada M5S 3H6

Correspondence e-mail: chealkim@sunt.ac.kr, ymeekim@ewha.ac.kr

Key indicators

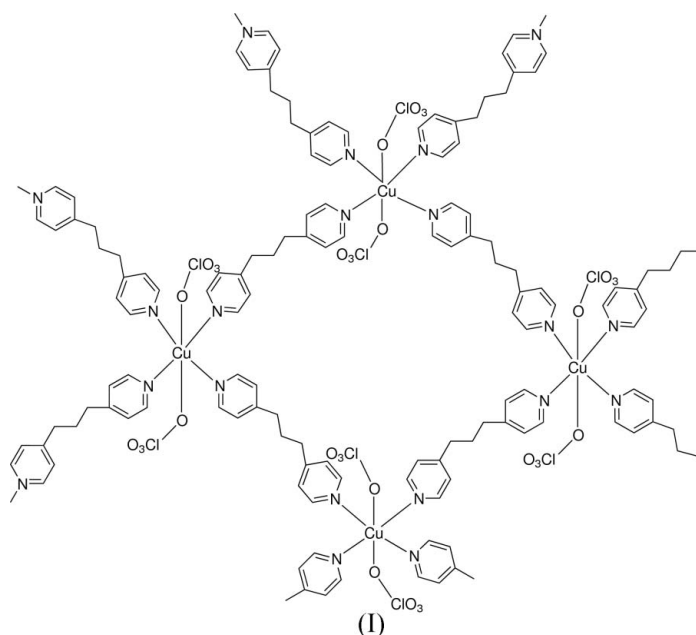
Single-crystal X-ray study
 $T = 150\text{ K}$
 Mean $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$
 R factor = 0.057
 wR factor = 0.159
 Data-to-parameter ratio = 14.0

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, $[\text{Cu}(\text{ClO}_4)_2(\text{C}_{13}\text{H}_{14}\text{N}_2)_2]_n$, 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 $\text{Cu}-\text{N}$ bonds are in the range 2.014 (4)–2.031 (4) \AA , while the long axial $\text{Cu}-\text{O}$ distances range from 2.434 (3) to 2.548 (3) \AA .

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.



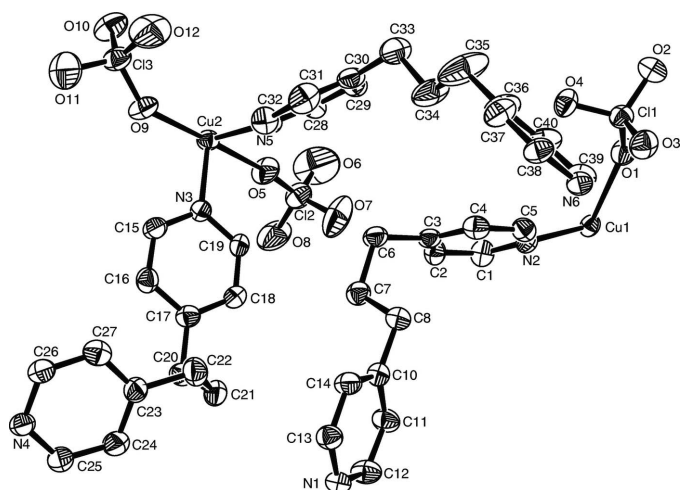


Figure 1
The asymmetric unit of (I), showing 50% probability displacement ellipsoids (H atoms omitted for clarity).

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(ClO₄)₂·6H₂O (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(ClO₄)₂(C₁₃H₁₄N₂)₂]

M_r = 658.96

Monoclinic, *P*2₁/*c*

a = 15.0179 (5) Å

b = 16.2881 (5) Å

c = 18.5719 (7) Å

β = 102.9642 (13)°

V = 4427.2 (3) Å³

Z = 6

D_x = 1.483 Mg m^{−3}

Mo Kα radiation

Cell parameters from 27195

reflections

θ = 2.6–27.5°

μ = 0.98 mm^{−1}

T = 150 (1) K

Block, violet

0.10 × 0.08 × 0.06 mm

Data collection

Bruker–Nonius KappaCCD

diffractometer

φ scans and ω scans with κ offsets

Absorption correction: multi-scan

(SORTAV; Blessing, 1995)

T_{min} = 0.689, *T_{max}* = 0.952

27195 measured reflections

7778 independent reflections

5253 reflections with *I* > 2σ(*I*)

R_{int} = 0.097

θ_{max} = 25.0°

h = −17 → 16

k = −18 → 19

l = −21 → 22

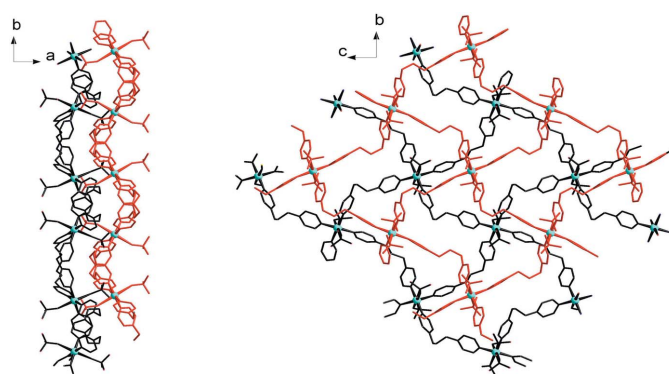


Figure 2
Structures of the two-dimensional sheets in (I). The red bonds represent a sheet containing Cu1, and the black bonds a sheet containing Cu2.

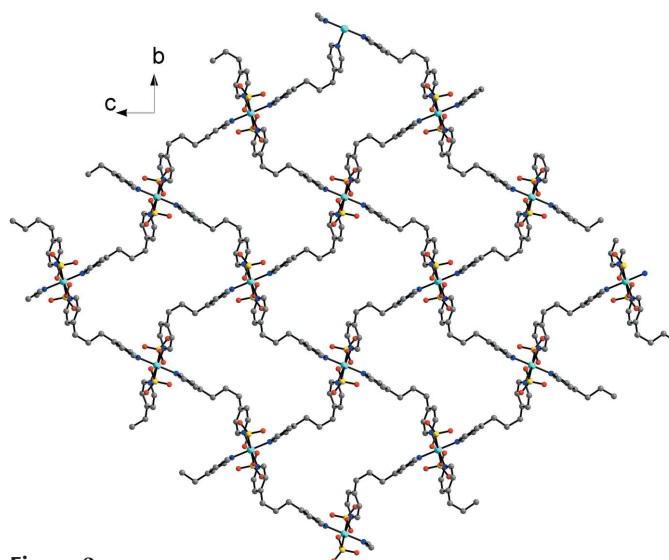


Figure 3
Two-dimensional sheet containing Cu1 atoms.

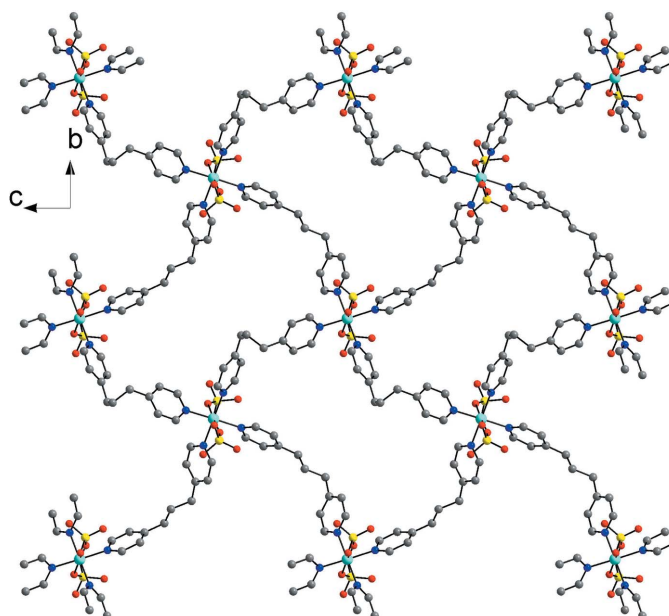


Figure 4
Two-dimensional sheet containing Cu2 atoms.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0775P)^2 + 2.2199P]$
$R[F^2 > 2\sigma(F^2)] = 0.057$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.159$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.03$	$\Delta\rho_{\max} = 0.46 \text{ e } \text{\AA}^{-3}$
7778 reflections	$\Delta\rho_{\min} = -0.68 \text{ e } \text{\AA}^{-3}$
557 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	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 $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$.

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*.

Financial support from the Korean Science and Engineering Foundation [R01-2005-000-10490-0(2005)] and the Korea Research Foundation (2002-070-C00053) is gratefully acknowledged.

References

- Balzani, V., Juris, A., Venturi, M., Campagna, S. & Serroni, S. (1996). *Chem. Rev.* **96**, 759–834.
- Barnett, S. A. & Champness, N. R. (2003). *Coord. Chem. Rev.* **246**, 145–168.
- Batten, S. R. & Robson, R. (1998). *Angew. Chem. Int. Ed.* **37**, 1460–1494.
- Blessing, R. H. (1995). *Acta Cryst.* **A51**, 33–38.
- Carlucci, L., Ciani, G., v. Gudenberg, D. W. & Proserpio, D. M. (1997). *Inorg. Chem.* **36**, 3812–3813.
- Hong, S. J., Ryu, J. Y., Lee, J. Y., Kim, C., Kim, S.-J. & Kim, Y. (2004). *Dalton Trans.* pp. 2697–2700.
- Leininger, S., Olenyuk, B. & Stang, P. S. (2000). *Chem. Rev.* **100**, 853–908.
- Nonius (2003). *Collect.* Nonius BV, Delft, The Netherlands.
- Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
- Plater, M. J., St J. Foreman, M. R., Gelbrich, T. & Hursthouse, M. B. (2000). *J. Chem. Soc. Dalton Trans.* pp. 1995–2000.
- Sheldrick, G. M. (2001). *SHELXTL/PC*. Version 6.12, Windows NT Version. Bruker AXS Inc., Madison, USA.