

Hexaaquacopper(II) diperchlorate dihydrate

Xin-Hua Li,^{a*} Feng-Yi Xia,^b
Hong-Ping Xiao^a and
Mao-Lin Hu^a

^aSchool of Chemistry and Materials Science,
Wenzhou Normal College, Zhejiang, Wenzhou
325027, People's Republic of China, and

^bSchool of Biological and Environmental
Sciences, Wenzhou Normal College, Zhejiang,
Wenzhou 325027, People's Republic of China

Correspondence e-mail: xhli@wznc.zj.cn

Key indicators

Single-crystal X-ray study

$T = 273\text{ K}$

Mean $\sigma(\text{Cl}-\text{O}) = 0.003\text{ \AA}$

R factor = 0.032

wR factor = 0.105

Data-to-parameter ratio = 14.1

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

In the title compound, $[\text{Cu}(\text{H}_2\text{O})_6](\text{ClO}_4)_2 \cdot 2\text{H}_2\text{O}$, six water molecules are coordinated to one Cu^{2+} ion, which lies on an inversion centre. The geometry around the Cu^{2+} ion is that of an octahedron. The coordinated water molecules, uncoordinated water molecules and perchlorate ions are linked by hydrogen bonds into a network structure.

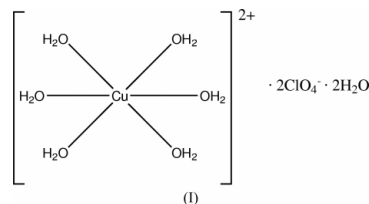
Received 19 January 2004

Accepted 28 January 2004

Online 7 February 2004

Comment

In the synthesis of crystal structures by design, the assembly of molecular units in predefined arrangements is a key goal (Desiraju, 1995, 1997; Braga *et al.*, 1998). Directional intermolecular interactions are the primary tools in achieving this goal and hydrogen bonding is currently the best among them (Zaworotko, 1997; Braga & Grepioni, 2000). We report here the structure of hexaaquacopper(II) diperchlorate dihydrate, (I).



The asymmetric unit of (I) consists of one half of a $[\text{Cu}(\text{H}_2\text{O})_6]^{2+}$ cation, a ClO_4^- anion and a water molecule. The copper cation lies on an inversion centre, and the geometry around the Cu^{2+} ion is that of an octahedron, with bonds to six water molecules (Fig. 1 and Table 1). The coordinated water molecules, uncoordinated water molecules and perchlorate ions interact through hydrogen bonds (Fig. 2), generating a three-dimensional network.

Experimental

Copper chloride dihydrate (0.06 g, 0.3 mmol) was dissolved in water (10 ml) and the solution was mixed with a dimethylformamide solution (10 ml) of 2,2'-dithiosalicylic acid (0.08 g, 0.2 mmol) and

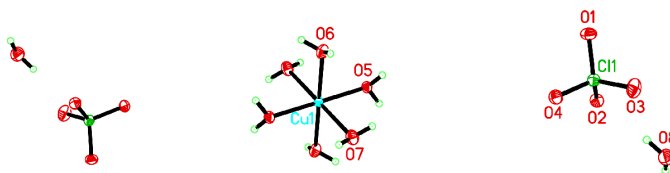


Figure 1

ORTEPII (Johnson, 1976) plot of (I), showing 50% probability displacement ellipsoids. Only the contents of the asymmetric unit are labelled.

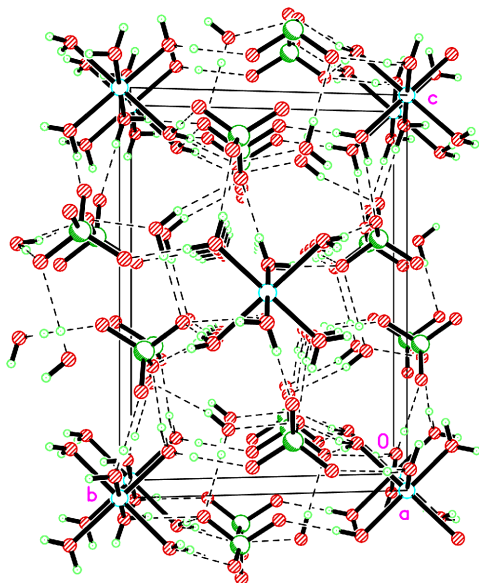


Figure 2
A view of the hydrogen-bonded three-dimensional network in (I).

ammonium pyrrolidine dithiocarbamate (0.06 g, 0.4 mmol). Perchloric acid (0.4 ml) was added dropwise. The reaction mixture was filtered; blue prism-shaped crystals were separated from the solution after about a month. As shown by the crystal structure analysis, the dithiosalicylate and ammonium pyrrolidine dithiocarbamate entities were not incorporated into the product.

Crystal data

[Cu(H ₂ O) ₆](ClO ₄) ₂ ·2H ₂ O	$D_x = 1.954 \text{ Mg m}^{-3}$
$M_r = 406.57$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 3539 reflections
$a = 6.2908 (3) \text{ \AA}$	$\theta = 2.8\text{--}25.2^\circ$
$b = 12.4043 (6) \text{ \AA}$	$\mu = 2.05 \text{ mm}^{-1}$
$c = 9.2181 (5) \text{ \AA}$	$T = 273 (2) \text{ K}$
$\beta = 106.146 (2)^\circ$	Prism, pale blue
$V = 690.94 (6) \text{ \AA}^3$	$0.60 \times 0.52 \times 0.29 \text{ mm}$
$Z = 2$	

Data collection

Bruker SMART APEX area-detector diffractometer	1244 independent reflections
φ and ω scans	1214 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$R_{\text{int}} = 0.016$
$T_{\text{min}} = 0.290$, $T_{\text{max}} = 0.555$	$\theta_{\text{max}} = 25.2^\circ$
3539 measured reflections	$h = -5 \rightarrow 7$
	$k = -14 \rightarrow 14$
	$l = -10 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0626P)^2 + 0.7948P]$
$R[F^2 > 2\sigma(F^2)] = 0.033$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.105$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.17$	$\Delta\rho_{\text{max}} = 0.47 \text{ e \AA}^{-3}$
1244 reflections	$\Delta\rho_{\text{min}} = -0.60 \text{ e \AA}^{-3}$
88 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (\AA , $^\circ$).

Cu1—O5	1.969 (2)	Cu1—O7	2.202 (2)
Cu1—O6	2.084 (2)		
O5—Cu1—O5 ⁱ	180	O5 ⁱ —Cu1—O7	90.58 (9)
O5—Cu1—O6 ⁱ	91.09 (9)	O6 ⁱ —Cu1—O7	88.68 (9)
O5—Cu1—O6	88.91 (9)	O6—Cu1—O7	91.32 (9)
O6 ⁱ —Cu1—O6	180	O7—Cu1—O7 ⁱ	180
O5—Cu1—O7	89.42 (9)		

Symmetry code: (i) $2 - x, -y, -z$.

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
O5—H5A \cdots O2 ⁱⁱ	0.82	1.92	2.733 (3)	174
O5—H5 \cdots O1 ⁱⁱⁱ	0.82	1.87	2.686 (3)	174
O6—H6A \cdots O3 ^{iv}	0.81	1.90	2.716 (3)	176
O6—H6 \cdots O4 ^v	0.82	1.94	2.748 (3)	172
O7—H7A \cdots O4 ⁱⁱ	0.81	2.02	2.820 (3)	168
O7—H7 \cdots O2 ^{vi}	0.81	2.02	2.825 (3)	172
O8—H8 \cdots O1 ^{vii}	0.83	2.19	2.984 (4)	162
O8—H8A \cdots O2	0.83	2.04	2.860 (4)	176

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

H atoms were located in a difference map and were made to ride on their parent O atoms, with $O\text{—}H = 0.81\text{--}0.83 \text{ \AA}$ and $U_{\text{iso}} = 1.5U_{\text{eq}}(O)$.

Data collection: SMART (Bruker, 2002); cell refinement: SMART; data reduction: SAINT (Bruker, 2002); program(s) used to solve structure: SHELXTL (Bruker, 2002); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL and ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXTL.

The authors thank the Wenzhou S&T Project of China (No. S2003A008) and '551' Distinguished Person Foundation of Wenzhou.

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