

Poly[hexaaquacopper(II) [di- μ_3 -sulfato-disodiate(I)]]Wen Wu,^{a,b} J.-M. Xie,^{b*} D.-P. Xie^a and Y.-W. Xuan^a^aDepartment of Chemistry, Zhou Kou Normal University, 466001, People's Republic of China, and ^bDepartment of Chemistry, Jiangsu University, Zhenjiang 212003, People's Republic of China

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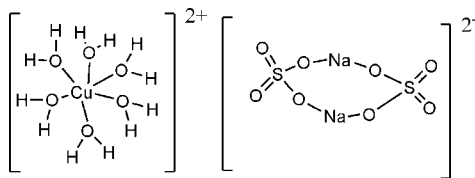
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Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(\text{Cu}-\text{O}) = 0.003$ Å; R factor = 0.036; wR factor = 0.092; data-to-parameter ratio = 11.7.

The title compound, $\{[\text{Cu}(\text{H}_2\text{O})_6][\text{Na}_2(\text{SO}_4)_2]\}_n$, has been prepared under mild hydrothermal conditions and has been structurally characterized. It exhibits a structure in which the inorganic frameworks are three-dimensional, participating in extensive hydrogen bonding. Copper occupies a special position ($\bar{1}$). The Na atom is coordinated by five O atoms of four sulfates [Na—O distances are between 2.825 (3) and 2.983 (3) Å]. The four O atoms of the sulfate ligand are coordinated to four Na atoms, the sulfate ligands coordinating in a chelating/bridging tetradentate mode.

Related literature

For the structure of $[\text{C}_6\text{H}_{18}\text{N}_2]_{0.5}[\text{Fe}(\text{SO}_4)_2(\text{H}_2\text{O})_2]$, see: Fu *et al.* (2006)



Experimental

Crystal data

 $[\text{Cu}(\text{H}_2\text{O})_6][\text{Na}_2(\text{SO}_4)_2]$ $M_r = 409.74$ Monoclinic, $P2_1/c$ $a = 6.2345$ (12) Å $b = 12.333$ (3) Å $c = 9.1822$ (18) Å $\beta = 105.56$ (3)° $V = 680.1$ (3) Å³ $Z = 2$ Mo $K\alpha$ radiation $\mu = 2.04$ mm⁻¹ $T = 291$ (2) K

0.20 × 0.17 × 0.17 mm

Data collection

Rigaku R-Axis IV diffractometer

Absorption correction: multi-scan

(SADABS; Sheldrick, 2004)

 $T_{\min} = 0.607$, $T_{\max} = 0.709$

2371 measured reflections

1322 independent reflections

1257 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.026$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.036$ $wR(F^2) = 0.092$ $S = 1.09$

1322 reflections

113 parameters

4 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.51$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.42$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O2}-\text{H2F}\cdots\text{O4}^{\text{i}}$	0.90 (3)	1.915 (15)	2.790 (3)	166 (4)
$\text{O3}-\text{H3F}\cdots\text{O6}^{\text{ii}}$	0.80 (5)	1.89 (5)	2.674 (4)	167 (5)
$\text{O1}-\text{H1F}\cdots\text{O5}^{\text{iii}}$	0.90 (3)	1.82 (3)	2.719 (4)	175 (5)
$\text{O1}-\text{H1E}\cdots\text{O7}^{\text{iv}}$	0.80 (5)	1.96 (5)	2.759 (4)	173 (4)
$\text{O2}-\text{H2E}\cdots\text{O7}$	0.90 (4)	1.93 (4)	2.800 (4)	164 (5)
$\text{O3}-\text{H3E}\cdots\text{O4}$	0.89 (3)	1.83 (3)	2.712 (3)	174 (4)

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

Data collection: *PROCESS* (Rigaku, 1996); cell refinement: *PROCESS*; data reduction: *PROCESS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *TEXSAN* (Molecular Structure Corporation, 1997); software used to prepare material for publication: *TEXSAN*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2054).

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