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Triaqua(1,10-phenanthroline)sulfatocopper(II) monohydrate

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In the title compound, $[Cu(SO_4)(C_{12}H_8N_2)(H_2O)_3]\cdot H_2O$, the Cu^{II} centre exhibits a slightly distorted *cis*-CuN_2O_4 octahedral coordination defined by two N atoms from a 1,10-phenanthroline molecule, one O atom from a sulfato dianion and three O atoms from coordinated water molecules.

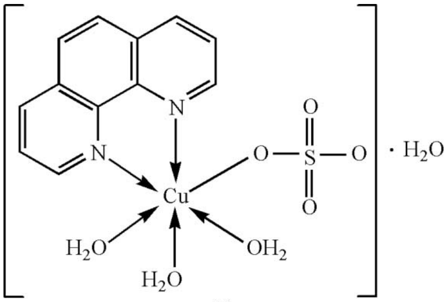
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.030
wR factor = 0.090
Data-to-parameter ratio = 11.4

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

Comment

1,10-Phenanthroline (phen) and its derivatives have been used widely in the construction of supramolecular architectures by way of metal–organic coordination (Chen & Liu, 2002; Xu *et al.*, 2003; Yu & Zhang, 2006; Wang *et al.*, 2007). As a continuation of these studies, we now report the crystal structure of the title complex, (I).



(I)

As illustrated in Fig. 1, the Cu^{II} ion is surrounded by two N atoms from one phen ligand and four O atoms from three H_2O molecules and one sulfate, forming a distorted *cis*-CuN_2O_4 octahedron (Table 1). A strong intramolecular O—H···O hydrogen bond occurs, as well as intermolecular links (Table 2).

Experimental

,10-Phenanthroline (0.05 g, 0.25 mmol) was dissolved in a water–DMF mixture (1:1 *v*/*v*, 50 ml), and $CuSO_4\cdot 5H_2O$ (0.04 g, 0.25 mmol) was added to the solution. The resulting mixture was stirred at room temperature for 3 h and filtered. Blue single crystals of (I) were obtained from the solution after several weeks.

Crystal data

$[Cu(SO_4)(C_{12}H_8N_2)(H_2O)_3]\cdot H_2O$
M_r = 411.87
Triclinic, $P\overline{1}$
a = 7.9908 (7) Å
b = 8.5918 (7) Å
c = 11.5799 (9) Å
α = 91.934 (1)°
β = 92.149 (1)°
γ = 104.319 (1)°
V = 769.02 (11) Å^3
Z = 2
D_x = 1.779 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.60 mm^{-1}
T = 295 (2) K
Prism, blue
0.36 × 0.28 × 0.16 mm

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Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.596$, $T_{\max} = 0.784$

3923 measured reflections
2754 independent reflections
2681 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.010$
$\theta_{\max} = 25.3°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.090$
$S = 1.12$
2754 reflections
241 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0488P)^2 + 0.9465P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.36$ e Å^{-3}
$\Delta\rho_{\min} = -0.75$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1*W*	2.0559 (18)	Cu1—N1	2.081 (2)
Cu1—O2*W*	2.0619 (18)	Cu1—O3*W*	2.1122 (19)
Cu1—N2	2.068 (2)	Cu1—O1	2.1323 (18)
N2—Cu1—N1	80.27 (8)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O3	0.845 (10)	1.799 (10)	2.637 (3)	172 (3)
O1*W*—H1*W*2···O4$^{\rm i}$	0.843 (10)	1.922 (13)	2.753 (3)	168 (3)
O2*W*—H2*W*1···O2$^{\rm ii}$	0.848 (10)	1.905 (12)	2.740 (3)	168 (3)
O2*W*—H2*W*2···O3$^{\rm i}$	0.844 (10)	1.927 (11)	2.768 (3)	174 (3)
O3*W*—H3*W*1···O4*W*	0.844 (10)	1.964 (14)	2.787 (3)	165 (3)
O3*W*—H3*W*2···O4*W*$^{\rm iii}$	0.85 (3)	2.008 (15)	2.814 (3)	160 (3)
O4*W*—H4*W*1···O3$^{\rm iv}$	0.84 (3)	1.957 (15)	2.777 (3)	165 (4)
O4*W*—H4*W*2···O4$^{\rm v}$	0.85 (3)	1.91 (3)	2.734 (3)	166 (3)

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

The carbon-bound H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The O-bound H atoms were located in a difference map and refined with a distance restraint of O—H 0.85 (1) Å and with $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm O})$.

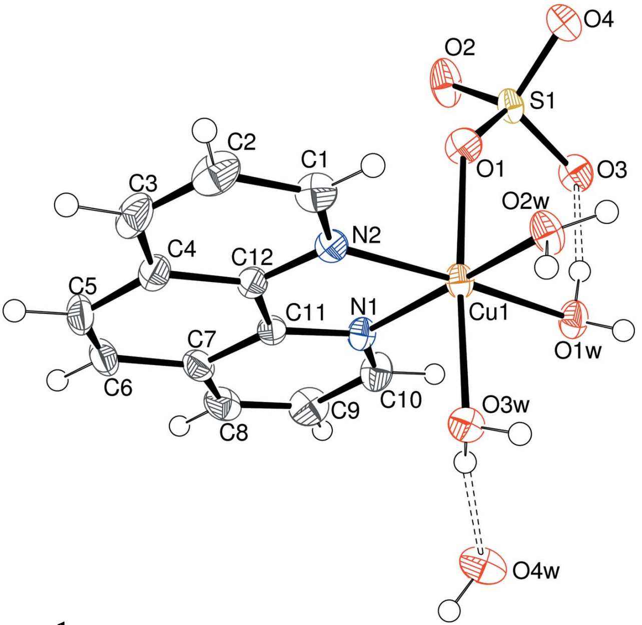

Figure 1
The asymmetric unit of (I), showing 50% probability displacement ellipsoids. Double dashed lines indicate hydrogen bonds.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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References

Bruker (1998). *SMART*, *SAINT* and *SHELXTL* Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, X.-M. & Liu, D.-F. (2002). *Chem. Eur. J.* **8**, 4811–4817.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Wang, H.-Y., Gao, S., Hou, L.-H. & Zhao, J.-G. (2007). *Acta Cryst.* E**63**, m7–m8.
Xu, L., Wang, E.-B., Peng, J. & Huang, R.-D. (2003). *Inorg. Chem. Commun.* **6**, 740–743.
Yu, C.-H. & Zhang, R.-C. (2006). *Acta Cryst.* E**62**, m1758–m1759.