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Triaqua(1,10-phenanthroline)sulfatocadmium(II)

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Hydrothermal reaction of $3CdSO_4{\cdot}8H_2O$ and phenanthroline (phen) in aqueous methanol resulted in the title mononuclear cadmium compound, $[Cd(SO_4)(C_{12}H_8N_2)(H_2O)_3]$. The coordination geometry around the Cd^{II} atom is distorted octahedral, in which one of the sulfate O atoms and an aqua ligand occupy the axial positions. Intermolecular O—H···O hydrogen bonds lead to the formation of a two-dimensional layer structure.

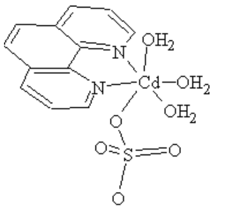
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.015 Å
R factor = 0.043
wR factor = 0.109
Data-to-parameter ratio = 11.3

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

Comment

The design and synthesis of novel inorganic–organic hybrid coordination complexes have attracted the attention of many chemists in recent years owing to their potential application, such as selective guest absorption (Gardner *et al.*, 1995), gas storage (Li *et al.*, 1999), and heterogeneous catalysis (Dong *et al.*, 2000). In the past years, cadmium complexes have been synthesized and characterized (Harvey *et al.*, 2000). In this paper, we report the structure of the title compound, (I), a new cadmium coordination compound.



(I)

The Cd atom is six-coordinated by two N atoms from phenanthroline, three O atoms from water molecules and one

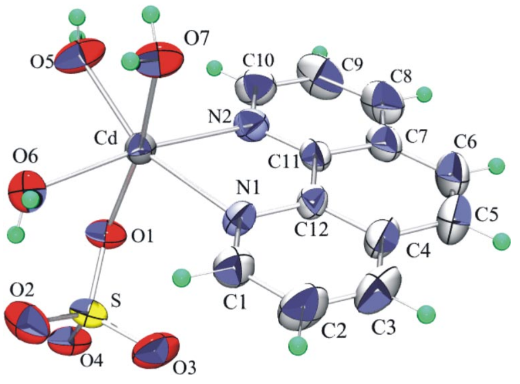


Figure 1
A view of the molecular structure of (I), showing 50% displacement ellipsoids for non-H atoms.

O atom from the sulfate ion (Fig. 1). The coordination geometry of the Cd^{II} atom can be regarded as distorted octahedral (Table 1), in which sulfate atom O1 and water atom O7 occupy the axial positions, while the equatorial plane is formed by N1, N2, O5 and O6. Through O—H···O hydrogen bonds, the crystal structure extends into a two-dimensional framework (Fig. 2).

Experimental

A mixture of $3CdSO_4{\cdot}8H_2O$ (0.2 mmol, 0.15 g), 1,10-phenanthroline (0.2 mmol, 0.04 g) and H_2O-EtOH (2:1 *v*/*v*, 15 ml) was sealed in a 25 ml Teflon-lined stainless-steel reactor and heated to 453 K for 72 h. After cooling, colorless crystals of the title compound, (I), were obtained (yield 68%).

Crystal data

$[Cd(SO_4)(C_{12}H_8N_2)(H_2O)_3]$
$M_r = 442.71$
Orthorhombic, $P2_12_12_1$
$a = 8.1620\ (5)$ Å
$b = 9.7458\ (6)$ Å
$c = 19.5727\ (11)$ Å
$V = 1556.91\ (16)$ Å^3
$Z = 4$
$D_x = 1.889$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 104 reflections
$\theta = 2.1$–25.1°
$\mu = 1.57$ mm^{-1}
$T = 293\ (2)$ K
Block, light yellow
0.36 × 0.18 × 0.04 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.416$, $T_{max} = 0.939$
5071 measured reflections
2500 independent reflections
2357 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 25.1°$
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 8$
$l = -20 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.109$
$S = 1.07$
2500 reflections
221 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 5.0252P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.73$ e Å^{-3}
$\Delta\rho_{min} = -1.22$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0049 (8)
Absolute structure: Flack (1983), 896 Friedel pairs
Flack parameter = −0.05 (5)

Table 1
Selected geometric parameters (Å, °).

Cd—O5	2.255 (6)	Cd—O7	2.303 (6)
Cd—O6	2.301 (5)	Cd—N2	2.325 (6)
Cd—O1	2.303 (5)	Cd—N1	2.327 (6)
O5—Cd—O6	93.3 (3)	O1—Cd—N2	91.9 (2)
O5—Cd—O1	92.9 (2)	O7—Cd—N2	98.1 (3)
O6—Cd—O1	82.8 (2)	O5—Cd—N1	161.2 (3)
O5—Cd—O7	87.3 (2)	O6—Cd—N1	102.1 (2)
O6—Cd—O7	87.2 (2)	O1—Cd—N1	99.7 (2)
O1—Cd—O7	170.0 (2)	O7—Cd—N1	82.7 (2)
O5—Cd—N2	93.0 (3)	N2—Cd—N1	72.7 (2)
O6—Cd—N2	171.9 (3)		

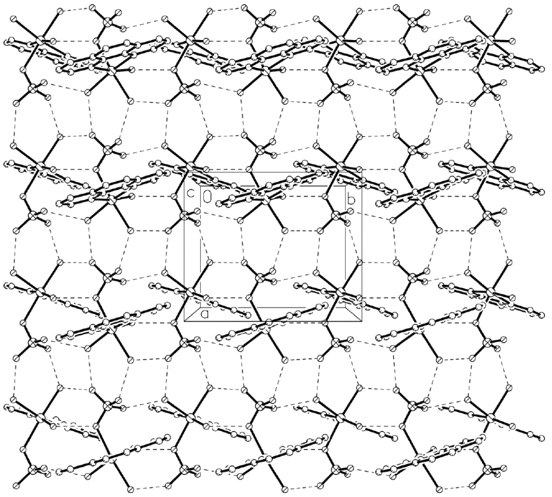


Figure 2
The two-dimensional structure of (I), formed through hydrogen bonding.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*A*···O4^{i}	0.82	1.95	2.736 (6)	160
O5—H5*C*···O2^{ii}	0.89 (14)	2.01 (10)	2.825 (6)	151 (4)
O6—H6*A*···O2	0.82	1.93	2.706 (6)	158
O6—H6*C*···O1^{iii}	0.89 (13)	1.87 (10)	2.737 (6)	164 (4)
O7—H7*A*···O3^{i}	0.82	1.97	2.674 (7)	151
O7—H7*B*···O4^{iii}	0.75 (9)	2.03 (10)	2.744 (6)	161 (3)

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

One H of each water molecule (H5*C*, H6*C* and H7*B*) was refined isotropically; the other H atoms were fixed. The positions of the H atoms bonded to C atoms were generated geometrically (C—H = 0.96 Å), assigned isotropic displacement parameters, and allowed to ride on their parent C atoms before the final cycle of least-squares refinement.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1994); program(s) used to solve structure: *SHELXTL* (Siemens, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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