Bis(1,10-phenanthroline-$\kappa^2 N,N'$)(sulfato-$\kappa^2 O,O'$)cadmium(II) 1,2-ethanediol solvate

Wen-Jie Lu,* Kai-Long Zhong and Yi-Min Zhu

Department of Chemical and, Environmental Engineering, Wuyi University, Jiangmen, Guangdong Province, People's Republic of China

Correspondence e-mail: wjlu_56@yahoo.com.cn

In the structure of the title compound, [Cd(SO$_4$)(C$_{12}$H$_8$N$_2$)$_2$]·-C$_2$H$_6$O$_2$, the [Cd(SO$_4$)(C$_{12}$H$_8$N$_2$)$_2$] and C$_2$H$_6$O$_2$ entities are connected by hydrogen bonding. The formula unit lies on a special position of site symmetry 2. The Cd^{II} centre is coordinated by four N atoms from two chelating 1,10-phenanthroline ligands and two O atoms from the bidentate sulfate ligand in a distorted octahedral geometry. The two chelating NCCN groups subtend a dihedral angle of 74.50 (9)°.

Comment

The sulfate ion, as a second ligand, has been found to be versatile when generating mixed-ligand complexes with d^{10} metal centres. It can act as a monodentate, bidentate or bidentate-bridging ligand, giving rise to monomeric, dimeric or polymeric structures in many complexes (Harvey *et al.*, 2000; 2003; Li *et al.*, 2003; Paul *et al.*, 2002). As such, the coordination modes can be tailored by introducing different neutral ligands into the complexes. The title compound, (I), was obtained unintentionally during an attempt to synthesize a mixed-ligand complex of Cd^{II} with 1,10-phenanthroline (phen) and 1,2-bis(2-pyridyl)ethylene *via* a solvothermal reaction. Here, we present the crystal structure of (I), which is isomorphous with the recently reported cobalt(II) structure (Zhong *et al.*, 2006).

(I)
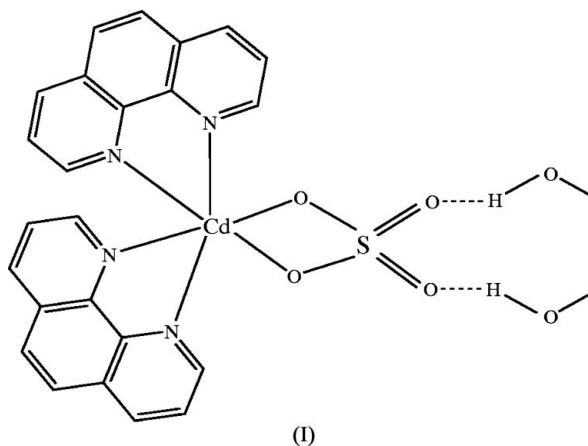
Other Cd–phen complexes with a monodentate sulfate ligand (Li *et al.*, 2003) or with a bidentate-bridging sulfate ligand (Harvey *et al.*, 2000) have been synthesized and characterized structurally by X-ray diffraction. Many other mixed-ligand cadmium complexes containing bidentate sulfate ligands (Harvey *et al.*, 2003; Paul *et al.*, 2002) have also been synthesized and reported. The title complex represents an addition to such complexes.

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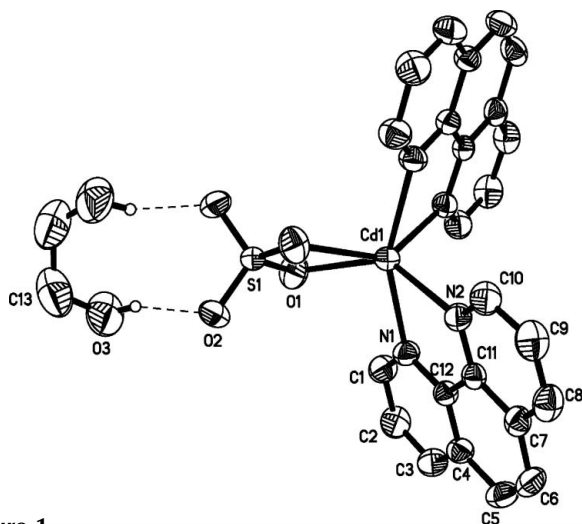
Figure 1
The structure of (I), showing the atom-numbering scheme and with displacement ellipsoids drawn at the 50% probability level. Dashed lines represent O—H···O interactions. H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry code for unlabelled atoms: $1 - x$, y, $\frac{1}{2} - z$.]

The metal complex and solvent components of (I) (Fig. 1) are held together by hydrogen bonding. A twofold rotation axis passes through the Cd and S atoms, and also through the centre of the solvent C—C bond. In the complex molecule, each Cd^{II} centre is coordinated by four N atoms from two chelating phen ligands and two O atoms from a bidentate sulfate ligand in a distorted octahedral geometry (Table 1). The geometry of the phen and sulfate ligands is in good agreement with those observed in many cadmium complexes. The Cd—N bond distances [2.327 (2)–2.343 (2) Å] are in good accord with those reported in six-coordinate Cd–phen complexes, e.g. $[Cd(phen)_2(H_2O)_2](C_4H_2O_4)\cdot 4H_2O$, (II) [2.338 (2)–2.383 (2) Å; Yang et al., 2003]. The N—Cd—N bite angle and the dihedral angle between the two chelating NCCN groups are also similar to those found in (II). The Cd—O bond distance [2.361 (2) Å] and O—Cd—O bite angle [59.98 (9)°] are close to those found in the cadmium complex $[H_3N(CH_2)_3NH_3][Cd_2(H_2O)_2(SO_4)_3]$ [2.334 (5)–2.545 (6) Å and 57.9 (2)°, respectively; Paul et al., 2002].

Experimental

The title compound, as pale-yellow block-shaped crystals, was obtained by a procedure similar to that described previously by Zhong et al. (2006), using $3Cd(SO_4)_2\cdot 8H_2O$ instead of $Co(SO_4)_2\cdot 7H_2O$.

Crystal data

Data collection

Bruker SMART CCD 1K area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
$T_{min} = 0.719$, $T_{max} = 0.823$
8598 measured reflections
3101 independent reflections
2710 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 28.3°$
$h = -24 \rightarrow 12$
$k = -16 \rightarrow 16$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.077$
$S = 1.09$
3101 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0348P)^2 + 1.3354P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.327 (2)	S1—O1	1.4841 (18)
Cd1—N2	2.343 (2)	O3—C13	1.372 (5)
Cd1—O1	2.361 (2)	C13—C13^i	1.460 (10)
S1—O2	1.4548 (19)		
N1—Cd1—N2	71.91 (7)	O1^i—S1—O1	105.37 (16)
O1—Cd1—O1^i	59.98 (9)	O3—C13—C13^i	117.3 (4)
O2^i—S1—O2	110.38 (17)		

Symmetry code: (i) $-x + 1$, y, $-z + \frac{1}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2	0.82	2.01	2.807 (3)	164

The H atoms of the phen ligand were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms of the 1,2-ethanediol solvent were located in a difference map and then allowed to ride on their parent atoms, with C—H = 0.97 and O—H = 0.82 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(O)$.

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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