Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Aqua[(benzothiazol-2-ylsulfanyl)acetato-κ*O*]-bis(1,10-phenanthroline-κ²*N*,*N*′)cadmium(**II**) nitrate monohydrate

He-Dong Bian, Fu-Ping Huang, Qing Yu and Hong Liang*

College of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin, Guangxi 541004, People's Republic of China

Correspondence e-mail:
bianhd@mailbox.gxnu.edu.cn

Received 7 December 2006
Accepted 20 December 2006

Key indicators

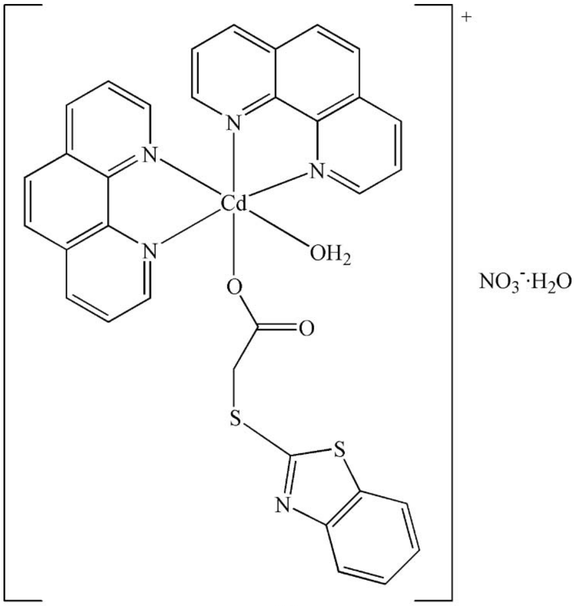
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.036
wR factor = 0.094
Data-to-parameter ratio = 12.7

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

In the title compound, $[Cd(C_9H_6NO_2S_2)(C_{12}H_8N_2)_2(H_2O)]NO_3\cdot H_2O$, the Cd atom is coordinated by four N atoms [Cd—N = 2.376 (3)–2.394 (3)Å] and two O atoms [Cd—O = 2.240 (2)–2.274 (3)Å] in a distorted octahedral geometry. The crystal structure exhibits intermolecular O—H···O hydrogen bonds and π–π stacking interactions.

Comment

The π–π stacking interaction correlates with electron transfer in some biological systems (Deisenhofer & Michel, 1989). In order to study its nature, a series of metal complexes with aromatic ligands has been synthesized, and their crystal structures have been determined (Su, Gu & Xu, 2005; Li *et al.*, 2005; Su, Zhang & Xu, 2005). As part of this ongoing work, the title compound, (I) (Fig. 1), has been prepared and structurally characterized.



(I)

In (I), the Cd(II) atom is coordinated by two bidentate 1,10-phenanthroline (phen) and one monodentate 2-benzothiazolylthioacetate ligands and one water molecule in a distorted octahedral geometry (Table 1). The Cd—N and Cd—O bond lengths agree well with those observed in analogous complexes (Huo *et al.*, 2005; Zhuo *et al.*, 2006). The mean planes of the two phen ligands make a dihedral angle of 102.9 (3)°.

The crystal packing (Fig. 2) exhibits intermolecular O—H···O hydrogen bonds (Table 2) and π–π stacking inter-

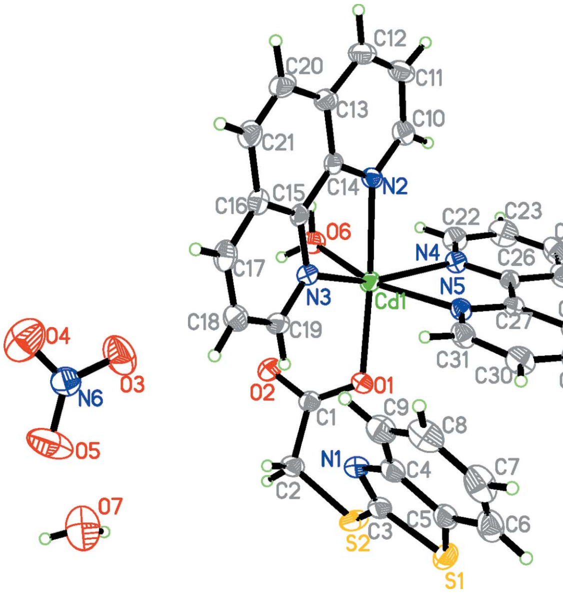


Figure 1
The asymmetric unit of (I) with the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level.

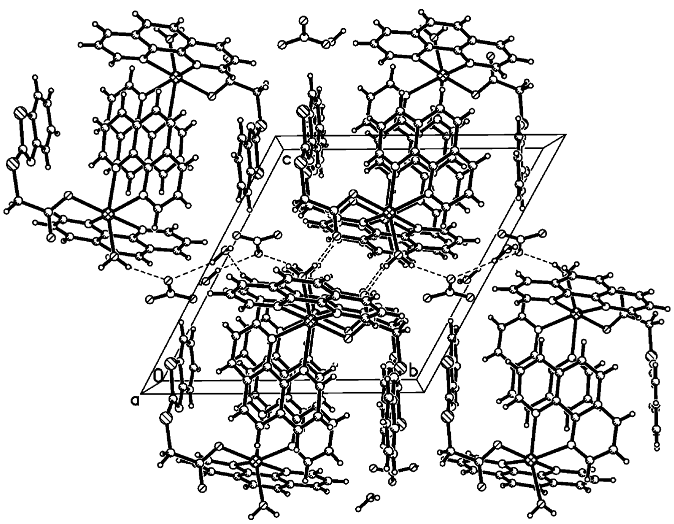


Figure 2
The crystal packing of (I), viewed down the *a* axis. The dashed lines denote hydrogen bonds.

actions. The centroids of the rings C25–C28/C32/C33 (*Cg*1), N4/C22–C26 (*Cg*2), C13–C16/C20/C21 (*Cg*3), N3/C15–C19 (*Cg*4), S1/N1/C3–C5 (*Cg*5) and C4–C9 (*Cg*6) make short contacts, *viz.* $Cg1\cdots Cg1^{i}$ 3.670 (3), $Cg1\cdots Cg2^{i}$ 3.799 (5), $Cg3\cdots Cg4^{ii}$ 3.729 (7), $Cg4\cdots Cg4^{ii}$ 3.740 (3) and $Cg6\cdots Cg5^{iii}$ 3.723 (6)Å [symmetry codes: (i) $-x + 2, -y + 1, -z + 2$; (ii) $-x + 1, -y + 1, -z + 1$; (iii) $-x + 1, -y, -z + 2$].

Experimental

2-Benzothiazolylthioacetic acid was prepared according to a literature method (Mei *et al.*, 1998). For the preparation of the title complex, 2-benzothiazolylthioacetic acid (0.225 g, 1 mmol), $Cd(NO_3)_2\cdot 4H_2O$ (0.31 g, 1 mmol), phen (0.20 g, 1 mmol) and $KHCO_3$ (0.10 g, 1 mmol) were dissolved in a water–ethanol solution (20 ml, 1:1). The solution was stirred for 3 h at room temperature and then filtered. Colourless block-shaped crystals were obtained from the filtrate after 4 d.

Crystal data

$[Cd(C_9H_6NO_2S_2)(C_{12}H_8N_2)_2(H_2O)]NO_3\cdot H_2O$
$M_r = 795.12$
Triclinic, $P\overline{1}$
$a = 9.545$ (2) Å
$b = 13.733$ (4) Å
$c = 14.150$ (4) Å
$\alpha = 61.742$ (2)°
$\beta = 82.225$ (3)°
$\gamma = 89.823$ (3)°
$V = 1614.8$ (7) Å^3
$Z = 2$
$D_x = 1.635$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.87$ mm^{-1}
$T = 298$ (2) K
Block, colourless
0.38 × 0.33 × 0.25 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.735$, $T_{max} = 0.813$
8450 measured reflections
5602 independent reflections
4439 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.0$°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.094$
$S = 1.00$
5602 reflections
442 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0474P)^2 + 0.3252P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.58$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.240 (2)	Cd1—N4	2.376 (3)
Cd1—O6	2.274 (3)	Cd1—N5	2.383 (3)
Cd1—N3	2.376 (3)	Cd1—N2	2.394 (3)
O1—Cd1—O6	108.46 (10)	N3—Cd1—N5	92.00 (10)
O1—Cd1—N3	93.32 (10)	N4—Cd1—N5	70.11 (10)
O6—Cd1—N3	104.53 (10)	O1—Cd1—N2	162.06 (10)
O1—Cd1—N4	103.36 (10)	O6—Cd1—N2	83.42 (10)
O6—Cd1—N4	90.47 (11)	N3—Cd1—N2	70.26 (10)
N3—Cd1—N4	152.86 (10)	N4—Cd1—N2	89.59 (10)
O1—Cd1—N5	80.97 (9)	N5—Cd1—N2	92.11 (10)
O6—Cd1—N5	160.14 (10)		

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O6—H34$\cdots$O2^{iv}	0.85	1.89	2.725 (4)	169
O6—H35$\cdots$O4^{ii}	0.85	2.04	2.852 (5)	159
O7—H36$\cdots$O4^{v}	0.85	2.03	2.860 (6)	167
O7—H37$\cdots$O4^{vi}	0.85	2.32	3.135 (7)	160

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

The H atoms of the water molecules were located in a difference Fourier map. The C-bound H atoms were positoned geometrically with C—H = 0.93Å. All H atoms were refined as riding with $U_{iso}(H) = 1.2U_{eq}$(parent atom).

m370 Bian *et al.* • $[Cd(C_9H_6NO_2S_2)(C_{12}H_8N_2)_2(H_2O)]NO_3\cdot H_2O$ *Acta Cryst.* (2007). E**63**, m369--m371

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, 1997); software used to prepare material for publication: *SHELXTL*.

We gratefully acknowledge the financial support of the Science Foundation of Guangxi, China, the Youth Science Foundation of Guangxi and the Teaching and Research Award Programme for Outstanding Young Teachers in Higher Education Institutions of MOE, China.

References

Bruker (1997). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (1998). *SMART* (Version 5.051) and *SAINT* (Version 5.01) and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Deisenhofer, J. & Michel, H. (1989). *EMBO J.* **8**, 2149–2154.

Huo, L.-H., Gao, S. & Ng, S. W. (2005). *Acta Cryst.* E**61**, m2357–m2358.

Li, H., Yin, K.-L. & Xu, D.-J. (2005). *Acta Cryst.* C**61**, m19–m21.

Mei, H.-M., Li, H.-P., Zhao, H.-T., Liu, S.-P. & Guo, D.-T. (1998). *J. HuNan Univ.* **25**, 33–36. (In Chinese.)

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Su, J.-R., Gu, J.-M. & Xu, D.-J.(2005). *Acta Cryst.* E**61**, m244–m246.

Su, J.-R., Zhang, L. & Xu, D.-J. (2005). *Acta Cryst.* E**61**, m939–m941.

Zhuo, X., Pan, Z.-R., Wang, Z.-W., Li, Y.-Z. & Zheng, H.-G. (2006). *Chin. J. Inorg. Chem.* **22**, 1847–1851.

Acta Cryst. (2007). E**63**, m369–m371 Bian *et al.* • $[Cd(C_9H_6NO_2S_2)(C_{12}H_8N_2)_2(H_2O)]NO_3\cdot H_2O$ **m371**