metal-organic papers

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.006 Å
R factor = 0.037
wR factor = 0.089
Data-to-parameter ratio = 12.3

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

Aquabis(1,10-phenanthroline)(3-sulfonatobenzoato)cadmium(II) tetrahydrate

In the title mononuclear complex, [Cd(C$_7$H$_4$O$_5$S)(C$_{12}$H$_8$N$_2$)$_2$-(H$_2$O)]·4H$_2$O, the Cd^{II} atom is coordinated in a capped trigonal–prismatic geometry by four N atoms and three O atoms. The 3-sulfonatobenzoate ligand chelates the Cd^{II} atom only *via* the carboxyl group. In the crystal structure, extensive O—H···O hydrogen bonds generate a three-dimensional network.

Comment

2- or 4-Sulfobenzoate metal complexes have shown interesting crystal structures (Fan, Xiao, Zhang & Zhu, 2004; Fan, Xiao, Zhang, Cai & Zhu, 2004; Xiao *et al.*, 2005; Zhang *et al.*, 2005) but are still fairly rare in the literature. In the related complex of 4-sulfobenzoic acid, cadmium, 1,10-phenanthroline and water, a dimer structure is formed (Fan *et al.*, 2005). However, in the title complex, (I), using 3-sulfobenzoate (3-sb) instead of 4-sulfobenzoate, a mononuclear structure is formed.

(I)
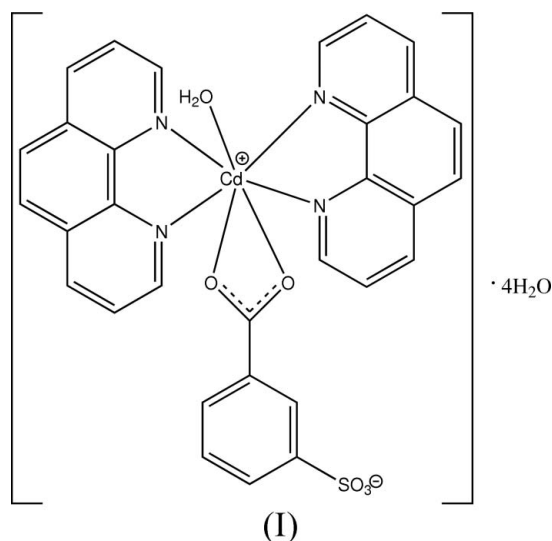
In (I), the Cd^{II} atom adopts a seven-coordinate geometry defined by four N atoms from two 1,10-phenanthroline ligands, two O atoms from the carboxylate group and one O atom from one water molecule (Fig. 1 and Table 1). The coordination around the Cd^{II} atom is best described as capped trigonal prismatic (Fig. 2), which is completely different from that of bis[diaqua(1,10-phenanthroline)(4-sulfonatobenzo-ato)cadmium(II)] (Fan *et al.*, 2005). The 3-sb ligand chelates to the Cd^{II} atom using the carboxylate group, while the sulfonate group is uncoordinated and is involved in hydrogen bonding with the coordinated and uncoordinated water molecules. In the crystal structure, molecules are linked *via* extensive O—
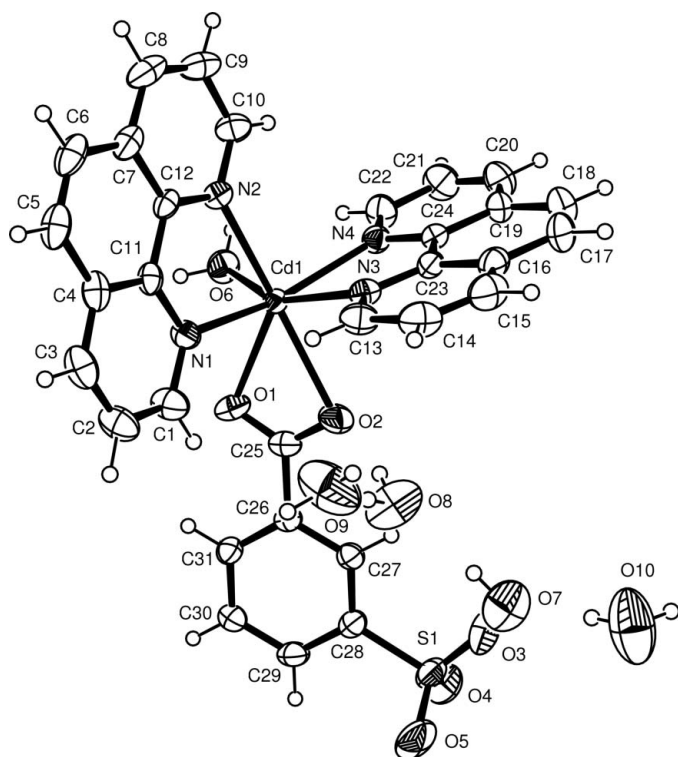
Figure 1
ORTEP-3 (Farrugia, 1997) view of (I), showing displacement ellipsoids drawn at the 40% probability level.

H···O intermolecular hydrogen bonds to give rise to a three-dimensional network (Table 2).

Experimental

A mixture of $Cd(CH_3COO)_2 \cdot 2H_2O$ (0.060 g, 0.23 mmol), sodium hydrogen 3-sulfobenzoate (0.046 g, 0.21 mmol), 1,10-phenanthroline hydrate (0.058 g, 0.29 mmol) and water (10 ml) was sealed in a 20 ml Teflon-lined stainless steel autoclave and heated at 423 K for 51 h. After cooling to room temperature, colorless plate-shaped crystals of (I) were obtained and collected by suction filtration.

Crystal data

$[Cd(C_7H_4O_5S)(C_{12}H_8N_2)_2(H_2O)]\cdot4H_2O$	$Z = 2$
$M_r = 763.05$	$D_x = 1.579$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 10.0335$ (10) Å	Cell parameters from 4655 reflections
$b = 11.8829$ (12) Å	$\theta = 2.3–25.6°$
$c = 14.3960$ (15) Å	$\mu = 0.81$ mm^{-1}
$\alpha = 77.925$ (1)°	$T = 295$ (2) K
$\beta = 74.887$ (1)°	Plate, colorless
$\gamma = 79.370$ (1)°	$0.25 \times 0.12 \times 0.04$ mm
$V = 1604.9$ (3) Å^3	

Data collection

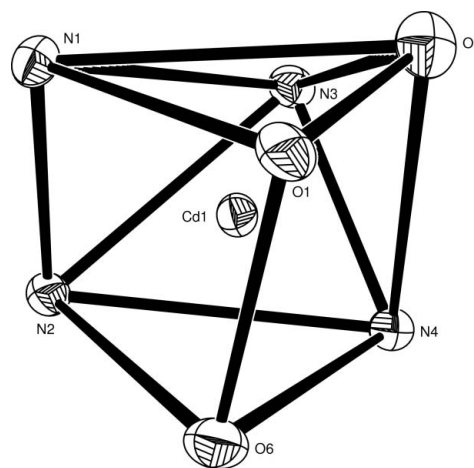|	
Bruker APEX area-detector diffractometer	5583 independent reflections
φ and ω scans	4992 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	$R_{int} = 0.028$
$T_{min} = 0.830$, $T_{max} = 0.968$	$\theta_{max} = 25.0°$
11638 measured reflections	$h = -11 \rightarrow 11$
	$k = -14 \rightarrow 14$
	$l = -17 \rightarrow 17$

Figure 2
A view of the capped trigonal–prismatic coordination of the Cd^{II} atom in (I).

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.037$	$+ 0.9145P]$
$wR(F^2) = 0.089$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
5583 reflections	$\Delta\rho_{max} = 0.92$ e Å^{-3}
454 parameters	$\Delta\rho_{min} = -0.70$ e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.420 (3)	Cd1—N2	2.384 (3)
Cd1—O2	2.474 (3)	Cd1—N3	2.400 (3)
Cd1—O6	2.377 (3)	Cd1—N4	2.361 (3)
Cd1—N1	2.387 (3)		
N4—Cd1—O6	85.51 (10)	O6—Cd1—O1	73.42 (9)
N4—Cd1—N2	94.21 (10)	N2—Cd1—O1	133.94 (9)
O6—Cd1—N2	84.66 (10)	N1—Cd1—O1	81.92 (9)
N4—Cd1—N1	153.72 (10)	N3—Cd1—O1	127.11 (9)
O6—Cd1—N1	112.17 (10)	N4—Cd1—O2	93.28 (9)
N2—Cd1—N1	69.47 (10)	O6—Cd1—O2	113.89 (10)
N4—Cd1—N3	70.30 (10)	N2—Cd1—O2	160.50 (9)
O6—Cd1—N3	154.22 (10)	N1—Cd1—O2	96.64 (9)
N2—Cd1—N3	88.28 (9)	N3—Cd1—O2	77.35 (9)
N1—Cd1—N3	88.22 (10)	O1—Cd1—O2	52.79 (9)
N4—Cd1—O1	122.92 (9)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6A···O1^i	0.85 (3)	1.95 (1)	2.792 (4)	168 (4)
O6—H6B···O5^{ii}	0.86 (1)	1.86 (2)	2.694 (4)	164 (5)
O8—H8A···O9	0.85 (3)	1.85 (3)	2.684 (5)	168 (5)
O9—H9A···O4^{iii}	0.85 (3)	1.96 (4)	2.793 (5)	166 (4)
O9—H9B···O10^{iv}	0.86 (3)	1.98 (3)	2.828 (6)	169 (4)
O8—H8B···O2	0.85 (3)	2.04 (3)	2.876 (5)	169 (5)
O7—H7A···O8	0.84 (4)	1.90 (4)	2.744 (5)	175 (5)
O10—H10B···O3^v	0.87 (3)	2.10 (3)	2.923 (6)	159 (3)
O10—H10A···O7	0.86 (3)	1.91 (3)	2.758 (5)	176 (5)
O7—H7B···O3	0.85 (3)	2.01 (2)	2.848 (5)	168 (4)

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

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H atoms on C atoms were placed in idealized positions and refined as riding atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. Water H atoms were located in difference Fourier maps and were refined with a distance restraint of O—H = 0.85 (1) Å and a fixed isotropic displacement parameter of $U_{iso}(H) = 0.08$ Å^2.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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