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Diaquabis(nicotinamide)bis(*o*-sulfobenzimidato-*N*)-cadmium(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.037
wR factor = 0.096
Data-to-parameter ratio = 14.7

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

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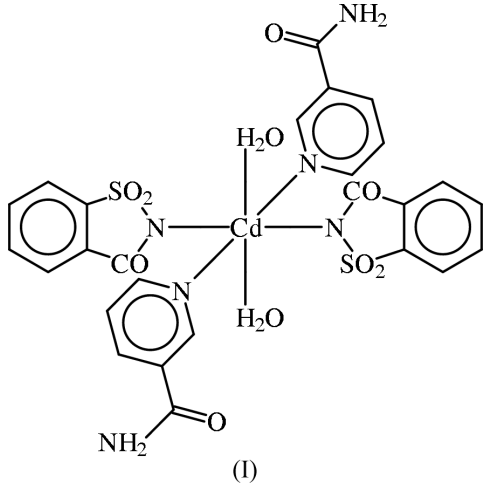
The Cd atom in the title compound, $[Cd(C_7H_4NO_3S)_2(C_6H_6N_2O)_2(H_2O)_2]$, lies on an inversion centre and is six-coordinate in an all-*trans* octahedral geometry. Hydrogen bonds involving a water molecule and the amido group of a nicotinamide ligand link adjacent molecules into layers.

Comment

The chemistry of the metal complexes of *o*-sulfobenzimide (saccharin) revolves around the bonding capabilities of the carbonyl, imido and sulfonyl donor sites (Jovanovski *et al.*, 1990; Jovanovski & Šoptrajanov, 1998; Naumov & Jovanovski, 2000*a*,*b*, 2001*a*,*b*). The metal *o*-sulfobenzimidates are themselves Lewis acids that furnish complexes with donor ligands, such as the *N*-heterocycles. Among these ligands, nicotinamide was selected for an examination of its ability to use its amido end to bind to cadmium; nicotinamide itself is a molecule that is found in a large number of biomolecules. A previous attempt to bind this ligand to the copper derivative resulted in its oxidation to nicotinic acid, which then complexed with the starting copper reagent (Naumov *et al.*, 2001). The corresponding cadmium reactant yielded the expected compound as a centrosymmetric water-coordinated complex. The bonding mode of the anion to the metal atom in the title compound, (I) (Fig. 1), contrasts with that suggested for the nicotinamide saccharinates $[M(C_6H_6N_2O)_2(H_2O)_4](C_7H_4NO_3S)_2$ (*M* = Co, Ni, Zn) and $[Cu(C_6H_6N_2O)_2(C_7H_4NO_3S)_2(H_2O)]$ (Çakir *et al.*, 2001).



(I)

Experimental

Tetraaquabis(*o*-sulfobenzimidato)cadmium(II) dihydrate was synthesized by treating cadmium chloride with sodium saccharinate

in water. The compound was isolated and then treated with two molar equivalents of nicotinamide in warm water. The crystals that separated from solution were collected and washed with acetone. They contained a small quantity of the starting cadmium compound, as implied by the CHN analytical values.

Crystal data

$[Cd(C_7H_4NO_3S)_2(C_6H_6N_2O)_2(H_2O)_2]$	D_x = 1.651 Mg m^{-3}
M_r = 757.03	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 8192 reflections
a = 7.6547 (1) Å	θ = 2.1–28.3°
b = 19.1163 (2) Å	μ = 0.92 mm^{-1}
c = 10.8285 (1) Å	T = 298 (2) K
β = 106.041 (1)°	Parallelepiped, colorless
V = 1522.83 (3) Å^3	0.34 × 0.26 × 0.16 mm
Z = 2	

Data collection

Siemens CCD area-detector diffractometer	3731 independent reflections
	3068 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.065
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)	θ_{max} = 28.3°
	$h = -10 \rightarrow 9$
T_{min} = 0.745, T_{max} = 0.867	$k = -24 \rightarrow 25$
10 747 measured reflections	$l = -8 \rightarrow 14$

Refinement

Refinement on F^2	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)]$ = 0.037	$w = 1/[\sigma^2(F_o^2) + (0.0431P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.096	$(\Delta/\sigma)_{max} < 0.001$
S = 0.99	$\Delta\rho_{max}$ = 0.51 e Å^{-3}
3731 reflections	$\Delta\rho_{min}$ = −1.48 e Å^{-3}
253 parameters	

Table 1
Selected geometric parameters (Å, °).

Cd1—O1*w*	2.323 (2)	S1—O2	1.424 (2)
Cd1—N1	2.343 (2)	S1—N1	1.626 (2)
Cd1—N2	2.371 (2)	O3—C7	1.233 (3)
S1—O1	1.441 (2)	N1—C7	1.355 (3)
O1*w*—Cd1—O1*w*^{i}	180.00 (1)	N1—Cd1—N2^{i}	91.51 (7)
O1*w*—Cd1—N1	86.51 (8)	N2—Cd1—N2^{i}	180.0
O1*w*—Cd1—N1^{i}	93.49 (8)	O2—S1—O1	115.1 (1)
O1*w*—Cd1—N2	92.50 (8)	N1—S1—C1	96.6 (1)
O1*w*—Cd1—N2^{i}	87.50 (8)	C7—N1—S1	111.5 (2)
N1—Cd1—N1^{i}	180.0	N1—C7—C6	112.7 (2)
N1—Cd1—N2	88.49 (7)		

Symmetry code: (i) $1-x, 1-y, 1-z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*2···O3	0.77 (5)	2.00 (5)	2.720 (3)	156 (5)
O1*w*—H1*w*1···O3^{i}	0.78 (4)	2.07 (5)	2.763 (3)	147 (4)
N3—H1*n*2···O1^{ii}	0.88 (4)	2.23 (4)	3.098 (4)	171 (3)
N3—H1*n*1···O4^{iii}	0.82 (3)	2.12 (3)	2.931 (4)	167 (3)

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

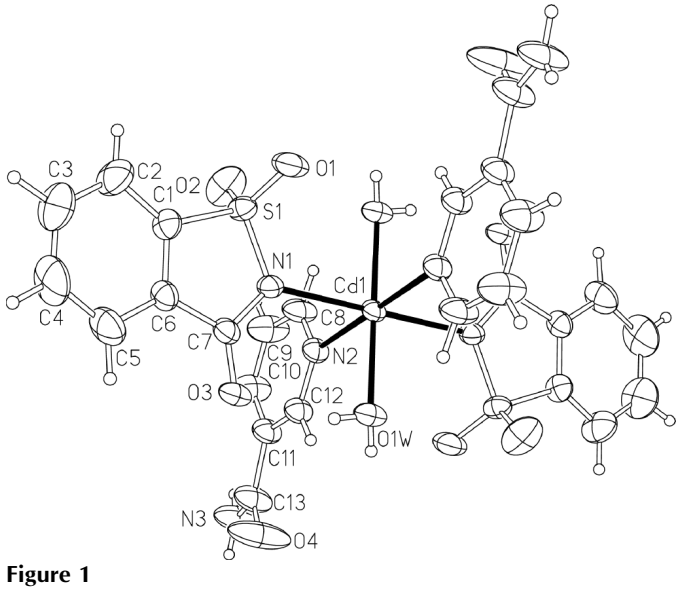


Figure 1
*ORTEP*II (Johnson, 1976) plot of the title compound at the 50% probability level. H atoms are shown as spheres of arbitrary radii.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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