Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Hexaaquacadmium(II) di-(*S*)-camphor-10-sulfonate

Jin-Sen Zhou,[a] Ji-Wen Cai[a] and Seik Weng Ng[b]*

[a]Department of Chemistry, Sun Yat-Sen University, Guangzhou 510275, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.044
wR factor = 0.116
Data-to-parameter ratio = 14.7

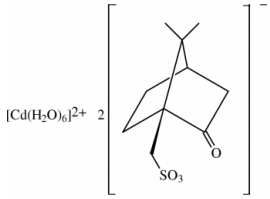
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 16 July 2003
Accepted 18 July 2003
Online 24 July 2003

The Cd atom in the title compound, $[Cd(H_2O)_6](C_{10}H_{15}O_4S)_2$, shows octahedral coordination. The cation is linked to the two anions by extensive hydrogen bonds.

Comment

Cadmium di-D-camphor-10-sulfonate was synthesized for its possible use as a gas absorbent, since a related dihydrate, cadmium 1,5-naphthalenedicarboxylate, exhibits selectivity for absorbing ammonia (Cai *et al.*, 2002). The D-camphor-10-sulfonate crystallizes as a hexaaqua complex, (I), which is isomorphous with the Ni^{II} analog, the structure of which has been described in detail (Henderson & Nicholson, 1995).



(I)

Experimental

Cadmium acetate (0.70 g, 1.5 mmol) and D-camphorsulfonic acid (0.40 g, 3 mmol) were dissolved in ethanol and the solution heated for several hours. Slow evaporation of the solvent afforded colorless crystals of the hexahydrate.

Crystal data

$[Cd(H_2O)_6](C_{10}H_{15}O_4S)_2$
M_r = 683.06
Monoclinic, $P2_1$
a = 11.775 (2) Å
b = 7.1711 (9) Å
c = 17.488 (2) Å
β = 93.914 (2)°
V = 1473.3 (3) Å^3
Z = 2
D_x = 1.540 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 963 reflections
θ = 2.8–27.1°
μ = 0.94 mm^{-1}
T = 298 (2) K
Parallelepiped, colorless
0.50 × 0.29 × 0.21 mm

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*: Sheldrick, 1996)
T_{min} = 0.650, T_{max} = 0.826
8977 measured reflections
5451 independent reflections
4624 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 27.1°
$h = -12 \rightarrow 15$
$k = -9 \rightarrow 8$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.116
S = 1.24
5451 reflections
370 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0631P)^2 + 0.1284P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −2.12 e Å^{-3}
Absolute structure: Flack (1983), 1973 Friedel pairs
Flack parameter = 0.00 (3)

Table 1
Selected geometric parameters (Å, °).

Cd1—O1*w*	2.244 (3)	Cd1—O4*w*	2.278 (5)
Cd1—O2*w*	2.221 (3)	Cd1—O5*w*	2.268 (6)
Cd1—O3*w*	2.270 (5)	Cd1—O6*w*	2.259 (6)
O1*w*—Cd1—O2*w*	176.8 (2)	O2*w*—Cd1—O6*w*	88.3 (2)
O1*w*—Cd1—O3*w*	88.6 (3)	O3*w*—Cd1—O4*w*	82.7 (3)
O1*w*—Cd1—O4*w*	91.6 (2)	O3*w*—Cd1—O5*w*	178.1 (3)
O1*w*—Cd1—O5*w*	92.5 (2)	O3*w*—Cd1—O6*w*	96.0 (1)
O1*w*—Cd1—O6*w*	88.8 (2)	O4*w*—Cd1—O5*w*	95.7 (1)
O2*w*—Cd1—O3*w*	90.3 (3)	O4*w*—Cd1—O6*w*	178.6 (2)
O2*w*—Cd1—O4*w*	91.2 (2)	O5*w*—Cd1—O6*w*	85.6 (3)
O2*w*—Cd1—O5*w*	88.7 (3)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O1	0.85 (1)	1.89 (4)	2.70 (1)	158 (9)
O1*w*—H1*w*2···O3^{i}	0.85 (1)	2.07 (6)	2.753 (9)	136 (8)
O2*w*—H2*w*1···O6^{ii}	0.85 (1)	1.92 (5)	2.69 (1)	149 (9)
O2*w*—H2*w*2···O5	0.85 (1)	1.91 (4)	2.71 (1)	155 (9)
O3*w*—H3*w*1···O2^{i}	0.85 (1)	2.07 (4)	2.802 (8)	145 (7)
O3*w*—H3*w*2···O6^{iii}	0.85 (1)	1.97 (3)	2.762 (7)	155 (7)
O4*w*—H4*w*2···O1^{iv}	0.85 (1)	2.07 (4)	2.805 (7)	144 (6)
O4*w*—H4*w*1···O7	0.86 (1)	1.98 (2)	2.832 (8)	172 (6)
O5*w*—H5*w*2···O3^{iv}	0.85 (1)	2.03 (2)	2.858 (7)	163 (6)
O5*w*—H5*w*1···O7^{ii}	0.86 (1)	2.04 (3)	2.849 (8)	157 (6)
O6*w*—H6*w*1···O2	0.85 (1)	1.98 (2)	2.801 (8)	163 (6)
O6*w*—H6*w*2···O5^{iii}	0.85 (1)	1.96 (1)	2.802 (7)	177 (6)

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

The H atoms of the water molecules were located and refined, subject to O—H = 0.85 (1) Å and H···H = 1.39 (1) Å. The carbon-bound H atoms were placed geometrically, and were allowed to ride on their parent atoms in the riding-model approximation. The displacement parameters of all H atoms were set at 1.2 times U_{eq} of the O and C atoms. The final difference Fourier map had a hole deeper than 2 e Å^{-3} at about 0.1 Å from Cd1.

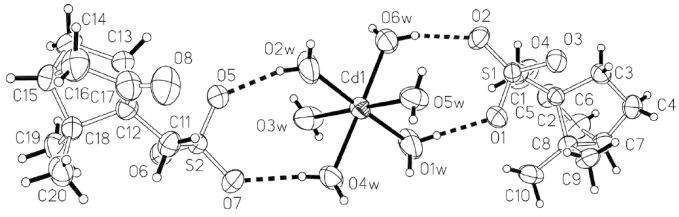


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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.

The authors thank the National Science Foundation of China (Grant No. 20271053), Sun Yat-Sen University and the University of Malaya for for supporting this work.

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