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Hexaaquacadmium(II) 2,2′-(azinodimethylidyne)dibenzenesulfonate dihydrate

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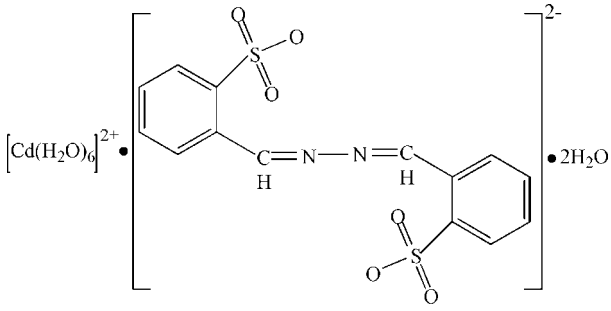
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.023; wR factor = 0.061; data-to-parameter ratio = 13.4.

In the title compound, $[Cd(H_2O)_6](C_{14}H_{10}O_6N_2S_2)\cdot 2H_2O$, the complete cation and anion are each generated by crystallographic inversion symmetry. In the crystal structure, the components form a three-dimensional network by way of O—H···O and O—H···N hydrogen bonds.

Related literature

For background to the properties and potential applications of organic–inorganic hybrid materials, see: Hagrman *et al.* (1998); Ranford *et al.* (1998).



Experimental

Crystal data

$[Cd(H_2O)_6](C_{14}H_{10}O_6N_2S_2)\cdot 2H_2O$
M_r = 622.89
Triclinic, $P\overline{1}$
a = 7.8329 (11) Å
b = 7.9824 (12) Å
c = 10.1010 (15) Å
α = 92.723 (1)°
β = 102.076 (2)°
γ = 105.924 (2)°
V = 590.19 (15) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.17 mm^{-1}
T = 298 (2) K
0.45 × 0.40 × 0.28 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.621, T_{max} = 0.735
3081 measured reflections
2041 independent reflections
1929 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.061
S = 1.06
2041 reflections
152 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—O5	2.2555 (18)	Cd1—O6	2.2947 (18)
Cd1—O4	2.2589 (17)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4A···O2^{i}	0.85	1.94	2.783 (3)	171
O4—H4B···O1^{ii}	0.85	2.03	2.872 (2)	174
O5—H5A···O1^{iii}	0.85	1.99	2.831 (3)	173
O5—H5B···O7^{iv}	0.85	2.00	2.843 (3)	173
O6—H6A···O7	0.85	2.08	2.881 (3)	157
O6—H6B···N1^{v}	0.85	2.15	2.993 (3)	169
O7—H7A···O3^{vi}	0.85	1.85	2.692 (3)	172
O7—H7B···O2^{iii}	0.85	2.21	3.002 (3)	156

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2858).

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Bruker (2000). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Hagrman, D., Hammond, R. P. & Haushalter, R. (1998). *Chem. Mater.* **10**, 2091–2096.
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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, m1625 [doi:10.1107/S1600536808039032]

Hexaaquacadmium(II) 2,2′-(azinodimethylidyne)dibenzenesulfonate dihydrate

Lian-Cai Du

S1. Comment

The design and synthesis of organic/inorganic hybrid materials have attracted intense attention in recent years owing to their potential practical applications, such as antitumor, antidiabetic, antitubercular activities, magnetism and catalysis [Ranford, *et al.*, 1998; Hagrman, *et al.*, 1998]. As part of our studies in this area, we now report the synthesis and crystal structure of the title compound, (I).

The Cd(II) centre is six-coordinate with six O donors of H_2O, and adopts distorted octahedral coordination (Table 1, Fig. 1). In the crystal, the molecules form a three-dimensional network by way of O—H···O and O—H···N hydrogen bonds (Table 2).

S2. Experimental

A solution of 1.0 mmol 2-formyl-benzenesulfonic acid-hydrazine and 1.0 mmol NaOH in 5 ml 95% ethanol was added to a solution of 0.5 mmol $Cd(CH_3COO)_2.4H_2O$ in 5 ml ethanol at room temperature. The mixture was refluxed for 4 h with stirring, then the resulting precipitate was filtered, washed, and dried *in vacuo* over P_4O_{10} for 48 h. Colourless blocks of (I) were obtained by slowly evaporating from methanol at room temperature.

S3. Refinement

H atom treatment??

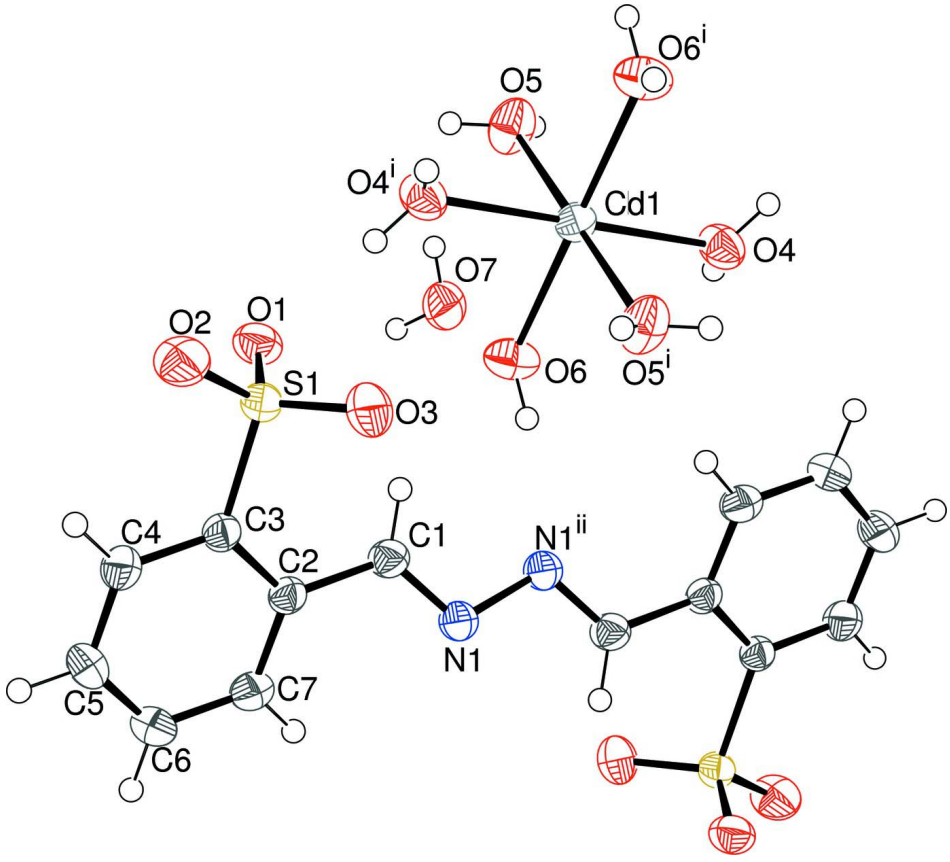

Figure 1

The molecular structure of (I) showing 50% displacement ellipsoids for the non-hydrogen atoms. Symmetry codes: (i) 1–x, 1–y, 1–z; (ii) 1–x, 1–y, –z.

Hexaaquacadmium(II) 2,2′-(azinodimethylidyne)dibenzenesulfonate dihydrate

Crystal data

$[Cd(H_2O)_6](C_{14}H_{10}O_6N_2S_2)\cdot 2H_2O$
$M_r = 622.89$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.8329\ (11)$ Å
$b = 7.9824\ (12)$ Å
$c = 10.1010\ (15)$ Å
$\alpha = 92.723\ (1)°$
$\beta = 102.076\ (2)°$
$\gamma = 105.924\ (2)°$
$V = 590.19\ (15)$ Å^3
$Z = 1$
$F(000) = 316$
$D_x = 1.753$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2719 reflections
$\theta = 2.7–28.3°$
$\mu = 1.17$ mm^{-1}
$T = 298$ K
Block, colourless
0.45 × 0.40 × 0.28 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.621$, $T_{max} = 0.735$
3081 measured reflections
2041 independent reflections
1929 reflections with $I > 2\sigma(I)$

R_{int} = 0.018
θ_{max} = 25.0°, θ_{min} = 2.1°
h = −9→9
k = −5→9
l = −11→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.061
S = 1.06
2041 reflections
152 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0313P)^2 + 0.2007P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.067 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cd1	0.5000	0.5000	0.5000	0.02922 (13)
N1	0.5732 (3)	0.5473 (3)	−0.0282 (2)	0.0336 (5)
O1	1.0298 (2)	0.6986 (2)	0.35433 (17)	0.0384 (4)
O2	1.1817 (3)	1.0036 (3)	0.35043 (19)	0.0465 (5)
O3	0.8508 (3)	0.8917 (3)	0.2790 (2)	0.0477 (5)
O4	0.2044 (2)	0.3385 (2)	0.45818 (18)	0.0406 (4)
H4A	0.1847	0.2342	0.4229	0.049*
H4B	0.1378	0.3362	0.5150	0.049*
O5	0.6085 (3)	0.3128 (3)	0.6297 (2)	0.0471 (5)
H5A	0.7201	0.3195	0.6358	0.057*
H5B	0.5490	0.2060	0.6283	0.057*
O6	0.5347 (3)	0.3561 (3)	0.30977 (19)	0.0448 (5)
H6A	0.5293	0.2485	0.3123	0.054*
H6B	0.4908	0.3730	0.2289	0.054*
O7	0.6167 (3)	0.0337 (3)	0.3703 (2)	0.0468 (5)
H7A	0.6908	−0.0043	0.3358	0.056*
H7B	0.6594	0.0466	0.4560	0.056*
S1	1.02370 (7)	0.85670 (8)	0.28844 (6)	0.02847 (16)
C1	0.7223 (3)	0.5998 (3)	0.0615 (2)	0.0303 (5)
H1	0.7234	0.5806	0.1517	0.036*

C2	0.8948 (3)	0.6913 (3)	0.0237 (2)	0.0265 (5)
C3	1.0408 (3)	0.8087 (3)	0.1183 (2)	0.0258 (5)
C4	1.2027 (3)	0.8863 (3)	0.0822 (3)	0.0348 (6)
H4	1.2984	0.9650	0.1451	0.042*
C5	1.2224 (4)	0.8469 (4)	−0.0476 (3)	0.0423 (6)
H5	1.3316	0.8989	−0.0717	0.051*
C6	1.0809 (3)	0.7311 (4)	−0.1414 (3)	0.0386 (6)
H6	1.0948	0.7044	−0.2284	0.046*
C7	0.9177 (3)	0.6542 (3)	−0.1061 (2)	0.0337 (5)
H7	0.8223	0.5768	−0.1701	0.040*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03192 (17)	0.02725 (17)	0.02920 (17)	0.01001 (10)	0.00609 (10)	0.00611 (10)
N1	0.0251 (10)	0.0408 (12)	0.0293 (11)	0.0001 (9)	0.0060 (8)	0.0066 (9)
O1	0.0449 (10)	0.0429 (10)	0.0318 (9)	0.0163 (8)	0.0123 (8)	0.0108 (8)
O2	0.0477 (11)	0.0433 (11)	0.0375 (10)	−0.0004 (9)	0.0074 (8)	−0.0093 (9)
O3	0.0429 (10)	0.0629 (13)	0.0486 (12)	0.0291 (10)	0.0168 (9)	0.0054 (10)
O4	0.0398 (10)	0.0394 (10)	0.0389 (10)	0.0022 (8)	0.0151 (8)	0.0000 (8)
O5	0.0416 (10)	0.0394 (11)	0.0614 (13)	0.0147 (9)	0.0069 (9)	0.0211 (9)
O6	0.0639 (12)	0.0415 (11)	0.0329 (10)	0.0200 (10)	0.0132 (9)	0.0038 (8)
O7	0.0447 (11)	0.0518 (12)	0.0501 (12)	0.0243 (9)	0.0123 (9)	−0.0007 (9)
S1	0.0288 (3)	0.0306 (3)	0.0257 (3)	0.0085 (2)	0.0063 (2)	0.0008 (2)
C1	0.0290 (12)	0.0316 (13)	0.0265 (12)	0.0036 (10)	0.0048 (10)	0.0033 (10)
C2	0.0251 (11)	0.0282 (12)	0.0260 (12)	0.0080 (9)	0.0044 (9)	0.0069 (9)
C3	0.0253 (11)	0.0268 (12)	0.0258 (12)	0.0086 (9)	0.0054 (9)	0.0055 (9)
C4	0.0259 (12)	0.0389 (14)	0.0329 (13)	0.0008 (10)	0.0040 (10)	0.0036 (11)
C5	0.0325 (13)	0.0565 (17)	0.0374 (15)	0.0052 (12)	0.0158 (11)	0.0127 (13)
C6	0.0401 (14)	0.0504 (16)	0.0287 (13)	0.0143 (12)	0.0131 (11)	0.0086 (12)
C7	0.0335 (13)	0.0382 (14)	0.0265 (12)	0.0087 (11)	0.0029 (10)	0.0021 (10)

Geometric parameters (Å, º)

Cd1—O5^{i}	2.2555 (18)	O6—H6B	0.8500
Cd1—O5	2.2555 (18)	O7—H7A	0.8499
Cd1—O4^{i}	2.2589 (17)	O7—H7B	0.8500
Cd1—O4	2.2589 (17)	S1—C3	1.783 (2)
Cd1—O6^{i}	2.2947 (18)	C1—C2	1.485 (3)
Cd1—O6	2.2947 (18)	C1—H1	0.9300
N1—C1	1.270 (3)	C2—C7	1.390 (3)
N1—N1^{ii}	1.431 (4)	C2—C3	1.403 (3)
O1—S1	1.4621 (19)	C3—C4	1.382 (3)
O2—S1	1.4523 (19)	C4—C5	1.384 (4)
O3—S1	1.4414 (18)	C4—H4	0.9300
O4—H4A	0.8500	C5—C6	1.377 (4)
O4—H4B	0.8500	C5—H5	0.9300
O5—H5A	0.8500	C6—C7	1.385 (4)

O5—H5B	0.8500	C6—H6	0.9300
O6—H6A	0.8499	C7—H7	0.9300
O5^{i}—Cd1—O5	180.0	O3—S1—O1	111.68 (12)
O5^{i}—Cd1—O4^{i}	95.45 (7)	O2—S1—O1	111.24 (12)
O5—Cd1—O4^{i}	84.55 (7)	O3—S1—C3	106.73 (11)
O5^{i}—Cd1—O4	84.55 (7)	O2—S1—C3	106.56 (11)
O5—Cd1—O4	95.45 (7)	O1—S1—C3	105.47 (10)
O4^{i}—Cd1—O4	180.0	N1—C1—C2	120.7 (2)
O5^{i}—Cd1—O6^{i}	89.86 (7)	N1—C1—H1	119.7
O5—Cd1—O6^{i}	90.14 (7)	C2—C1—H1	119.7
O4^{i}—Cd1—O6^{i}	90.19 (7)	C7—C2—C3	118.4 (2)
O4—Cd1—O6^{i}	89.81 (7)	C7—C2—C1	119.8 (2)
O5^{i}—Cd1—O6	90.14 (7)	C3—C2—C1	121.7 (2)
O5—Cd1—O6	89.86 (7)	C4—C3—C2	120.5 (2)
O4^{i}—Cd1—O6	89.81 (7)	C4—C3—S1	118.63 (17)
O4—Cd1—O6	90.19 (7)	C2—C3—S1	120.88 (17)
O6^{i}—Cd1—O6	180.0	C3—C4—C5	120.0 (2)
C1—N1—N1^{ii}	111.5 (2)	C3—C4—H4	120.0
Cd1—O4—H4A	113.7	C5—C4—H4	120.0
Cd1—O4—H4B	123.5	C6—C5—C4	120.3 (2)
H4A—O4—H4B	108.3	C6—C5—H5	119.9
Cd1—O5—H5A	116.0	C4—C5—H5	119.9
Cd1—O5—H5B	123.2	C5—C6—C7	120.0 (2)
H5A—O5—H5B	108.7	C5—C6—H6	120.0
Cd1—O6—H6A	116.9	C7—C6—H6	120.0
Cd1—O6—H6B	123.6	C6—C7—C2	120.8 (2)
H6A—O6—H6B	109.5	C6—C7—H7	119.6
H7A—O7—H7B	105.6	C2—C7—H7	119.6
O3—S1—O2	114.51 (12)		
N1^{ii}—N1—C1—C2	176.2 (2)	O3—S1—C3—C2	−47.1 (2)
N1—C1—C2—C7	−29.2 (4)	O2—S1—C3—C2	−169.90 (19)
N1—C1—C2—C3	154.3 (2)	O1—S1—C3—C2	71.8 (2)
C7—C2—C3—C4	0.5 (3)	C2—C3—C4—C5	−0.7 (4)
C1—C2—C3—C4	177.1 (2)	S1—C3—C4—C5	177.7 (2)
C7—C2—C3—S1	−177.85 (18)	C3—C4—C5—C6	0.3 (4)
C1—C2—C3—S1	−1.2 (3)	C4—C5—C6—C7	0.3 (4)
O3—S1—C3—C4	134.5 (2)	C5—C6—C7—C2	−0.5 (4)
O2—S1—C3—C4	11.7 (2)	C3—C2—C7—C6	0.1 (4)
O1—S1—C3—C4	−106.6 (2)	C1—C2—C7—C6	−176.6 (2)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*A*···O2^{iii}	0.85	1.94	2.783 (3)	171

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O5—H5*B*···O7^{v}	0.85	2.00	2.843 (3)	173
O6—H6*A*···O7	0.85	2.08	2.881 (3)	157
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Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*; (iii) *x*−1, *y*−1, *z*; (iv) −*x*+2, −*y*+1, −*z*+1; (v) −*x*+1, −*y*, −*z*+1; (vi) *x*, *y*−1, *z*.