

Cadmium sulfite hexahydrate revisited

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Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{S-O}) = 0.002$ Å; R factor = 0.018; wR factor = 0.040; data-to-parameter ratio = 13.9.

The present structural revision of the title compound, tetracadmium tetrasulfite hexahydrate, $[\text{Cd}_4(\text{SO}_3)_4(\text{H}_2\text{O})_5] \cdot \text{H}_2\text{O}$, is a low-temperature upgrade ($T = 100$ K and $R = 0.017$) of the original room-temperature structure reported by Kiers & Vos [*Cryst. Struct. Commun.* (1978), **7**, 399–403; $T = 293$ K and $R = 0.080$). The compound is a three-dimensional polymer with four independent cadmium centres, four sulfite anions and six water molecules, five of them coordinated to two cadmium centres and the remaining one an unbound solvent molecule which completes the asymmetric unit. There are two types of cadmium environment: CdO_8 (through four chelating sulfite ligands) and CdO_6 (by way of six monocoordinated ligands). The former groups form planar arrays [parallel to (001) and separated by half a unit cell translation along c], made up of chains running along [110] and $[\bar{1}10]$, respectively. These chains are, in turn, interconnected both in an intraplanar as well as in an interplanar fashion by the latter CdO_6 polyhedra into a tight three-dimensional framework. There is, in addition, an extensive network of hydrogen bonds, in which all 12 water H atoms act as donors and eight O atoms from all four sulfite groups and two water molecules act as acceptors.

Related literature

For related literature, see: Agre *et al.* (1981); Brown & Altermatt (1985); Elder *et al.* (1978); Harvey *et al.* (2006); Kiers & Vos (1978); Larsson & Kierkegaard (1969).

Experimental

Crystal data

$[\text{Cd}_4(\text{SO}_3)_4(\text{H}_2\text{O})_5] \cdot \text{H}_2\text{O}$	$V = 1731.82$ (11) Å ³
$M_r = 877.94$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 12.1406$ (3) Å	$\mu = 5.41$ mm ⁻¹
$b = 10.5485$ (3) Å	$T = 150$ (2) K
$c = 13.9329$ (4) Å	$0.24 \times 0.12 \times 0.08$ mm
$\beta = 103.93$ (1)°	

Data collection

Bruker SMART CCD area-detector diffractometer	31336 measured reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 2001)	3959 independent reflections
$T_{\min} = 0.40$, $T_{\max} = 0.64$	3922 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.017$	18 restraints
$wR(F^2) = 0.040$	All H-atom parameters refined
$S = 1.26$	$\Delta\rho_{\text{max}} = 0.70$ e Å ⁻³
3959 reflections	$\Delta\rho_{\text{min}} = -0.56$ e Å ⁻³
284 parameters	

Table 1

Selected bond lengths (Å).

Cd1—O13	2.2452 (18)	Cd2—O14	2.6091 (18)
Cd1—O32 ⁱ	2.2839 (18)	Cd2—O21	2.8126 (18)
Cd1—O22	2.3065 (18)	Cd3—O2W	2.215 (2)
Cd1—O21	2.4078 (17)	Cd3—O1W	2.2272 (19)
Cd1—O12	2.4542 (18)	Cd3—O3W	2.278 (2)
Cd1—O31	2.4752 (18)	Cd3—O31	2.3201 (17)
Cd1—O23	2.6544 (18)	Cd3—O12	2.3482 (18)
Cd1—O12 ^j	2.7665 (19)	Cd3—O11 ⁱⁱⁱ	2.3518 (18)
Cd2—O34	2.3311 (18)	Cd4—O34	2.2412 (18)
Cd2—O14 ⁱⁱ	2.3365 (18)	Cd4—O4W	2.2599 (18)
Cd2—O33	2.3440 (18)	Cd4—O5W	2.2601 (19)
Cd2—O11	2.3545 (18)	Cd4—O32 ^{iv}	2.2816 (18)
Cd2—O24 ⁱⁱ	2.4074 (18)	Cd4—O23 ^v	2.3203 (17)
Cd2—O23	2.4446 (18)	Cd4—O21	2.3571 (17)

Symmetry codes: (i) $-x + 1, -y, -z + 1$; (ii) $-x, -y + 1, -z + 1$; (iii) $-x + 1, -y + 1, -z + 1$; (iv) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$; (v) $x, -y + \frac{1}{2}, z + \frac{1}{2}$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1W—H1WA \cdots O13 ⁱ	0.82 (3)	1.88 (2)	2.693 (3)	170 (4)
O1W—H1WB \cdots O14 ^{vi}	0.82 (3)	1.93 (2)	2.679 (3)	151 (3)
O2W—H2WA \cdots O4W ^{iv}	0.82 (3)	1.93 (2)	2.719 (3)	162 (4)
O2W—H2WB \cdots O6W	0.82 (3)	1.95 (2)	2.681 (3)	149 (4)
O3W—H3WA \cdots O6W ^{vii}	0.82 (3)	2.02 (2)	2.833 (3)	172 (4)
O3W—H3WB \cdots O22 ^j	0.82 (3)	2.29 (2)	3.092 (3)	168 (4)
O4W—H4WA \cdots O22	0.82 (3)	1.87 (2)	2.651 (3)	159 (3)
O4W—H4WB \cdots O31 ^v	0.82 (3)	1.98 (2)	2.780 (3)	167 (3)
O5W—H5WA \cdots O33	0.82 (3)	2.05 (2)	2.848 (3)	167 (4)
O5W—H5WB \cdots O24 ^{viii}	0.82 (3)	1.92 (2)	2.708 (3)	162 (4)
O6W—H6WA \cdots O24 ^{ix}	0.82 (3)	2.16 (2)	2.876 (3)	146 (4)
O6W—H6WB \cdots O33 ^x	0.82 (3)	2.18 (2)	2.948 (3)	157 (4)

Symmetry codes: (i) $-x + 1, -y, -z + 1$; (iv) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$; (v) $x, -y + \frac{1}{2}, z + \frac{1}{2}$; (vi) $x + 1, y, z$; (vii) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (viii) $-x, y - \frac{1}{2}, -z + \frac{3}{2}$; (ix) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$; (x) $x + 1, -y + \frac{1}{2}, z + \frac{1}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2070).

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