Dirubidium tricadmium tetrakis(sulfate) pentahydrate

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Key indicators

Single-crystal X-ray study
 $T = 90\text{ K}$
Mean $\sigma(\text{S—O}) = 0.003\text{ \AA}$
 R factor = 0.022
 wR factor = 0.059
Data-to-parameter ratio = 11.0

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

The title compound, $\text{Rb}_2\text{Cd}_3(\text{SO}_4)_4 \cdot 5\text{H}_2\text{O}$, arose as an unexpected product during the attempted synthesis of an $\text{Rb}_2\text{Cd}_2(\text{SO}_4)_3$ potassium cadmium sulfate langbeinite. It has two layers, layer *A* containing Cd octahedra bridged by sulfate groups and layer *B* containing edge-shared Cd octahedra, with Rb atoms occupying interstitial positions. The layers are connected by way of Cd—O—S links.

Comment

The system $\text{Rb}_2\text{SO}_4\text{—CdSO}_4\text{—H}_2\text{O}$ was selected in an attempt to synthesize the langbeinite-type phase $\text{Rb}_2\text{Cd}_2(\text{SO}_4)_3$ by a slow evaporation method. Instead, the title compound, (I) (Fig. 1), a hydrated double salt, arose at 313 K.

The crystal structure of (I) is isomorphous with $\text{K}_2\text{Mn}_3(\text{SO}_4)_4 \cdot 5\text{H}_2\text{O}$ (Hidalgo *et al.*, 1996). The Cd atoms are octahedrally coordinated by O atoms of either sulfate groups or water molecules (Table 1).

Among the five water molecules, O18W bonds to two Cd atoms [$\text{Cd1—O18W—Cd2} = 114.72(12)^\circ$]. The four other water molecules are singly coordinated to Cd atoms. The crystal packing (Fig. 2) results in pseudo-layers parallel to the *bc* plane. Two types of layers, namely layer *A* formed by Cd octahedra bridged by sulfate groups and layer *B* containing edge-sharing Cd octahedra, occur. The pseudo-layers, which are connected by way of Cd—O—S bonds, repeat in a ...BABAB... fashion along the *a* axis, with the Rb cations in interstitial positions. A network of O—H...O bonds (Table 2) helps to consolidate the crystal packing.

Figure 1

View of the asymmetric unit of (I), showing 50% displacement ellipsoids. H atoms have been omitted for clarity.

Experimental

Colourless plates of (I) were synthesized by slow evaporation at 313 K of an aqueous solution containing equimolar amounts of Rb_2SO_4 and CdSO_4 . The temperature was maintained by a thermostat to control the evaporation rate.

Crystal data

$\text{Rb}_2\text{Cd}_3(\text{SO}_4)_4 \cdot 5\text{H}_2\text{O}$
 $M_r = 982.53$
 Monoclinic, $P2_1/c$
 $a = 19.6755$ (16) Å
 $b = 9.7855$ (8) Å
 $c = 9.9593$ (8) Å
 $\beta = 101.498$ (1)°
 $V = 1879.0$ (3) Å³
 $Z = 4$

$D_x = 3.473$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 890
 reflections
 $\theta = 0.9\text{--}28.7^\circ$
 $\mu = 9.06$ mm⁻¹
 $T = 90$ (2) K
 Plate, colourless
 $0.29 \times 0.16 \times 0.03$ mm

Data collection

Bruker SMART CCD
 diffractometer
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.189$, $T_{\max} = 0.755$
 13435 measured reflections

3434 independent reflections
 3296 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$
 $\theta_{\max} = 25.4^\circ$
 $h = -23 \rightarrow 23$
 $k = -11 \rightarrow 11$
 $l = -11 \rightarrow 11$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.059$
 $S = 1.10$
 3434 reflections
 311 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.024P)^2 + 6.4725P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 1.09$ e Å⁻³
 $\Delta\rho_{\min} = -0.58$ e Å⁻³

Table 1

Selected bond lengths (Å).

Rb1—O8	2.918 (3)	Rb2—O1	3.364 (3)
Rb1—O20W ⁱ	2.935 (3)	Rb2—O5 ^{iv}	3.457 (3)
Rb1—O9	2.960 (3)	Cd1—O6 ^{vii}	2.218 (3)
Rb1—O8 ⁱⁱⁱ	2.962 (3)	Cd1—O1	2.284 (3)
Rb1—O13 ⁱⁱⁱ	3.060 (3)	Cd1—O9 ^{vi}	2.288 (3)
Rb1—O16 ^{iv}	3.072 (3)	Cd1—O7 ^{vi}	2.295 (3)
Rb1—O6 ⁱⁱ	3.110 (3)	Cd1—O17W	2.304 (3)
Rb1—O12	3.147 (3)	Cd1—O18W	2.342 (3)
Rb1—O15 ^v	3.224 (3)	Cd2—O5	2.238 (3)
Rb1—O14 ⁱⁱⁱ	3.430 (3)	Cd2—O11 ^{vi}	2.243 (3)
Rb1—O14 ^v	3.538 (3)	Cd2—O4	2.277 (3)
Rb2—O15	2.777 (3)	Cd2—O19W	2.278 (3)
Rb2—O6 ^{iv}	2.824 (3)	Cd2—O10	2.316 (3)
Rb2—O11 ^{vi}	2.886 (3)	Cd2—O18W ^{iv}	2.316 (3)
Rb2—O10	2.992 (3)	Cd3—O13	2.264 (3)
Rb2—O7 ^{vii}	3.096 (3)	Cd3—O16 ^{iv}	2.265 (3)
Rb2—O8 ^{vii}	3.097 (3)	Cd3—O14 ⁱⁱⁱ	2.293 (3)
Rb2—O4	3.127 (3)	Cd3—O21W	2.304 (3)
Rb2—O9 ^{vi}	3.131 (3)	Cd3—O20W	2.331 (3)
Rb2—O19W ^{iv}	3.205 (3)	Cd3—O12	2.342 (3)

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

Figure 2
Packing diagram of (I).

Table 2

Hydrogen-bond geometry (Å, °).

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O17W—H17B $\cdots$ O3 ^{viii}	0.82	1.95	2.755 (4)	166
O18W—H18A $\cdots$ O2 ^{viii}	0.82	1.82	2.627 (4)	168
O18W—H18B $\cdots$ O3	0.82	1.79	2.599 (4)	169
O19W—H19A $\cdots$ O4 ^{vi}	0.82	2.02	2.807 (4)	162
O19W—H19B $\cdots$ O17W ^v	0.82	2.39	3.019 (4)	134
O20W—H20A $\cdots$ O21W ^{ix}	0.82	2.36	3.123 (4)	154
O20W—H20B $\cdots$ O13 ^{iv}	0.82	2.38	2.966 (4)	129
O20W—H20B $\cdots$ O14 ^{ix}	0.82	2.09	2.855 (4)	154
O21W—H21A $\cdots$ O5 ^{iv}	0.82	2.02	2.773 (4)	153
O21W—H21A $\cdots$ O15	0.82	2.50	2.914 (4)	112
O21W—H21B $\cdots$ O12 ^{iv}	0.82	1.93	2.751 (4)	174

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

Water H atoms were positioned geometrically ($\text{O—H} = 0.82$ Å) and refined as riding, with the constraint $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{carrier})$ applied. The highest electron-density peak is located 0.79 Å from atom S3.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2003).

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