Dirubidium tricadmium tetrakis(sulfate) pentahydrate

Diptikanta Swain and T. N. Guru Row*

Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, Karnataka, India

Correspondence e-mail:
ssctng@sscu.iisc.ernet.in

Key indicators

Single-crystal X-ray study
T = 90 K
Mean *σ*(S–O) = 0.003 Å
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, $Rb_2Cd_3(SO_4)_4·5H_2O$, arose as an unexpected product during the attempted synthesis of an $Rb_2Cd_2(SO_4)_3$ 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 interstial positions. The layers are connected by way of Cd—O—S links.

Comment

The system Rb_2SO_4–$CdSO_4$–H_2O was selected in an attempt to synthesize the langbeinite-type phase $Rb_2Cd_2(SO_4)_3$ 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 $K_2Mn_3(SO_4)_4·5H_2O$ (Hidalgon *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, O18*W* bonds to two Cd atoms [Cd1—O18*W*—Cd2 = 114.72 (12)°]. 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 octhedra 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 . . . *BABBAB* . . . 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.

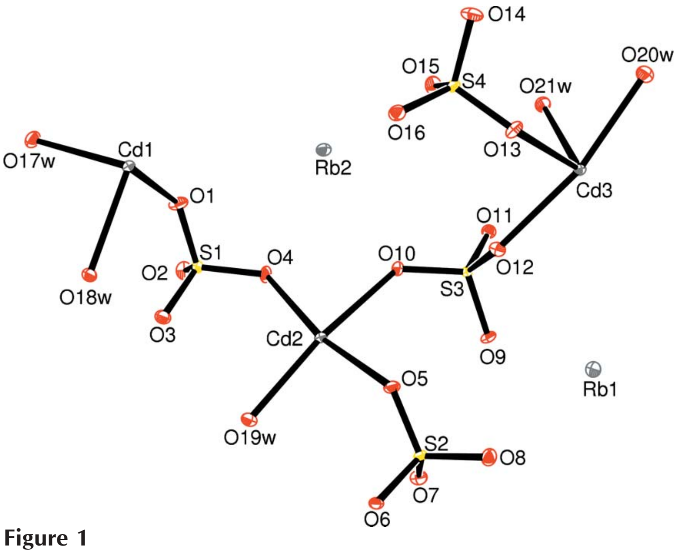

Figure 1
View of the asymmetric unit of (I), showing 50% displacement ellipsoids. H atoms have been omitted for clarity.

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

$Rb_2Cd_3(SO_4)_4 \cdot 5H_2O$
$M_r = 982.53$
Monoclinic, $P2_1/c$
$a = 19.6755\ (16)$ Å
$b = 9.7855\ (8)$ Å
$c = 9.9593\ (8)$ Å
$\beta = 101.498\ (1)^\circ$
$V = 1879.0\ (3)$ Å^3
$Z = 4$
$D_x = 3.473$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 890 reflections
$\theta = 0.9$–28.7°
$\mu = 9.06$ mm^{-1}
$T = 90\ (2)$ K
Plate, colourless
0.29 × 0.16 × 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 $I > 2\sigma(I)$
$R_{\rm int} = 0.031$
$\theta_{\max} = 25.4^\circ$
$h = -23 \rightarrow 23$
$k = -11 \rightarrow 11$
$l = -11 \rightarrow 11$

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—O20$W^{\rm i}$	2.935 (3)	Rb2—O5$^{\rm iv}$	3.457 (3)
Rb1—O9	2.960 (3)	Cd1—O6$^{\rm vii}$	2.218 (3)
Rb1—O8$^{\rm ii}$	2.962 (3)	Cd1—O1	2.284 (3)
Rb1—O13$^{\rm iii}$	3.060 (3)	Cd1—O9$^{\rm vi}$	2.288 (3)
Rb1—O16$^{\rm iv}$	3.072 (3)	Cd1—O7$^{\rm vi}$	2.295 (3)
Rb1—O6$^{\rm ii}$	3.110 (3)	Cd1—O17W	2.304 (3)
Rb1—O12	3.147 (3)	Cd1—O18W	2.342 (3)
Rb1—O15$^{\rm v}$	3.224 (3)	Cd2—O5	2.238 (3)
Rb1—O14$^{\rm iii}$	3.430 (3)	Cd2—O11$^{\rm vi}$	2.243 (3)
Rb1—O14$^{\rm v}$	3.538 (3)	Cd2—O4	2.277 (3)
Rb2—O15	2.777 (3)	Cd2—O19W	2.278 (3)
Rb2—O6$^{\rm iv}$	2.824 (3)	Cd2—O10	2.316 (3)
Rb2—O11$^{\rm vi}$	2.886 (3)	Cd2—O18$W^{\rm iv}$	2.316 (3)
Rb2—O10	2.992 (3)	Cd3—O13	2.264 (3)
Rb2—O7$^{\rm vii}$	3.096 (3)	Cd3—O16$^{\rm iv}$	2.265 (3)
Rb2—O8$^{\rm vii}$	3.097 (3)	Cd3—O14$^{\rm iii}$	2.293 (3)
Rb2—O4	3.127 (3)	Cd3—O21W	2.304 (3)
Rb2—O9$^{\rm vi}$	3.131 (3)	Cd3—O20W	2.331 (3)
Rb2—O19$W^{\rm iv}$	3.205 (3)	Cd3—O12	2.342 (3)

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

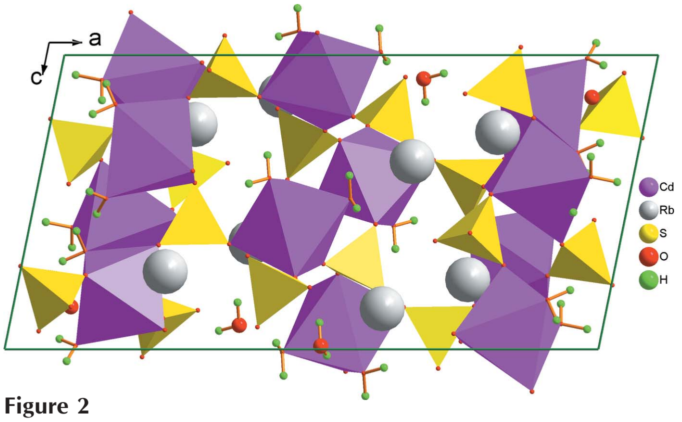

Figure 2
Packing diagram of (I).

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O17W—H17$B\cdots$O3$^{\rm viii}$	0.82	1.95	2.755 (4)	166
O18W—H18$A\cdots$O2$^{\rm viii}$	0.82	1.82	2.627 (4)	168
O18W—H18$B\cdots$O3	0.82	1.79	2.599 (4)	169
O19W—H19$A\cdots$O4$^{\rm vi}$	0.82	2.02	2.807 (4)	162
O19W—H19$B\cdots$O17$W^{\rm v}$	0.82	2.39	3.019 (4)	134
O20W—H20$A\cdots$O21$W^{\rm ix}$	0.82	2.36	3.123 (4)	154
O20W—H20$B\cdots$O13$^{\rm iv}$	0.82	2.38	2.966 (4)	129
O20W—H20$B\cdots$O14$^{\rm ix}$	0.82	2.09	2.855 (4)	154
O21W—H21$A\cdots$O5$^{\rm iv}$	0.82	2.02	2.773 (4)	153
O21W—H21$A\cdots$O15	0.82	2.50	2.914 (4)	112
O21W—H21$B\cdots$O12$^{\rm iv}$	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 (O—H = 0.82 Å) and refined as riding, with the constraint $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}$(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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