

Diptikanta Swain and  
T. N. Guru Row\*Solid State and Structural Chemistry Unit, Indian  
Institute of Science, Bangalore 560 012,  
Karnataka, IndiaCorrespondence e-mail:  
sctng@sscu.iisc.ernet.in

## Key indicators

Single-crystal X-ray study  
 $T = 90\text{ K}$   
Mean  $\sigma(\text{S}-\text{O}) = 0.003\text{ \AA}$   
 $R$  factor = 0.022  
 $wR$  factor = 0.059  
Data-to-parameter ratio = 11.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Dirubidium tricadmium tetrakis(sulfate)  
pentahydrate

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.

Received 21 June 2005

Accepted 4 July 2005

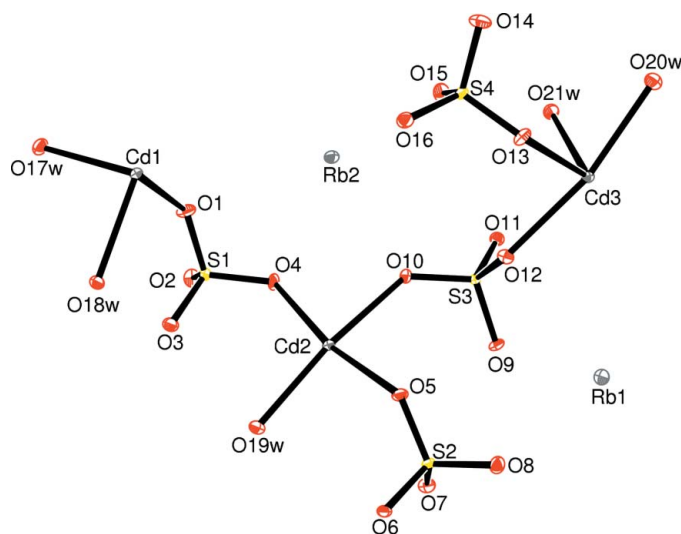
Online 13 July 2005

## 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  $\text{K}_2\text{Mn}_3(\text{SO}_4)_4 \cdot 5\text{H}_2\text{O}$  (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, 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 ...*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  $\text{Rb}_2\text{SO}_4$  and  $\text{CdSO}_4$ . 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) Å<sup>3</sup>  
 $Z = 4$

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

Data collection

Bruker SMART CCD diffractometer  
 $\varphi$  and  $\omega$  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  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.031$   
 $\theta_{\text{max}} = 25.4^\circ$   
 $h = -23 \rightarrow 23$   
 $k = -11 \rightarrow 11$   
 $l = -11 \rightarrow 11$

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  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 1.09$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.58$  e Å<sup>-3</sup>

Table 1

Selected bond lengths (Å).

Rb1—O8	2.918 (3)	Rb2—O1	3.364 (3)
Rb1—O20W <sup>i</sup>	2.935 (3)	Rb2—O5 <sup>iv</sup>	3.457 (3)
Rb1—O9	2.960 (3)	Cd1—O6 <sup>vii</sup>	2.218 (3)
Rb1—O8 <sup>ii</sup>	2.962 (3)	Cd1—O1	2.284 (3)
Rb1—O13 <sup>iii</sup>	3.060 (3)	Cd1—O9 <sup>vi</sup>	2.288 (3)
Rb1—O16 <sup>iv</sup>	3.072 (3)	Cd1—O7 <sup>vi</sup>	2.295 (3)
Rb1—O6 <sup>ii</sup>	3.110 (3)	Cd1—O17W	2.304 (3)
Rb1—O12	3.147 (3)	Cd1—O18W	2.342 (3)
Rb1—O15 <sup>v</sup>	3.224 (3)	Cd2—O5	2.238 (3)
Rb1—O14 <sup>iii</sup>	3.430 (3)	Cd2—O11 <sup>vi</sup>	2.243 (3)
Rb1—O14 <sup>v</sup>	3.538 (3)	Cd2—O4	2.277 (3)
Rb2—O15	2.777 (3)	Cd2—O19W	2.278 (3)
Rb2—O6 <sup>iv</sup>	2.824 (3)	Cd2—O10	2.316 (3)
Rb2—O11 <sup>vi</sup>	2.886 (3)	Cd2—O18W <sup>iv</sup>	2.316 (3)
Rb2—O10	2.992 (3)	Cd3—O13	2.264 (3)
Rb2—O7 <sup>vii</sup>	3.096 (3)	Cd3—O16 <sup>iv</sup>	2.265 (3)
Rb2—O8 <sup>vii</sup>	3.097 (3)	Cd3—O14 <sup>iii</sup>	2.293 (3)
Rb2—O4	3.127 (3)	Cd3—O21W	2.304 (3)
Rb2—O9 <sup>vi</sup>	3.131 (3)	Cd3—O20W	2.331 (3)
Rb2—O19W <sup>iv</sup>	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)  $x, y + 1, z$ .

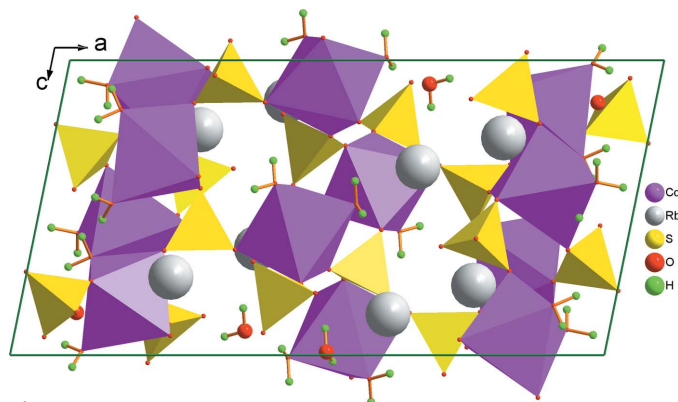


Figure 2  
Packing diagram of (I).

Table 2

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
O17W—H17B...O3 <sup>viii</sup>	0.82	1.95	2.755 (4)	166
O18W—H18A...O2 <sup>viii</sup>	0.82	1.82	2.627 (4)	168
O18W—H18B...O3	0.82	1.79	2.599 (4)	169
O19W—H19A...O4 <sup>vi</sup>	0.82	2.02	2.807 (4)	162
O19W—H19B...O17W <sup>v</sup>	0.82	2.39	3.019 (4)	134
O20W—H20A...O21W <sup>ix</sup>	0.82	2.36	3.123 (4)	154
O20W—H20B...O13 <sup>iv</sup>	0.82	2.38	2.966 (4)	129
O20W—H20B...O14 <sup>ix</sup>	0.82	2.09	2.855 (4)	154
O21W—H21A...O5 <sup>iv</sup>	0.82	2.02	2.773 (4)	153
O21W—H21A...O15	0.82	2.50	2.914 (4)	112
O21W—H21B...O12 <sup>iv</sup>	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  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{carrier})$  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).

The authors thank the Department of Science and Technology, India (IRHPA-DST), for providing the CCD facility at the Indian Institute of Science.

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