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$Rb_2Mn_2(SO_4)_3$, a new member of the langbeinite family

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The structure of a new langbeinite, dirubidium dimanganese trisulfate, $Rb_2Mn_2(SO_4)_3$, has been determined and is shown to have cubic symmetry akin to the other members of the langbeinite family. The sturucture contains SO_4 tetrahedra corner-linked to MnO_6 octahedra, generating a three-dimensional network. The Rb atoms are found in the cavities of this network.

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(S–O) = 0.002 Å
R factor = 0.013
wR factor = 0.038
Data-to-parameter ratio = 14.8

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

Comment

$Rb_2Mn_2(SO_4)_3$ belongs to the langbeinite family, having the general formula $A_2B_2(XO_4)_3$, where A = Rb, Li, NH_4, Tl, K or Cs, B = Mg, Ca, Mn, Fe, Co, Ni, Cu, Zn, Cd with X = S, Se or Mo. The name originates from the natural langbeinite $K_2Mg_2(SO_4)_3$, the crystal structure of which was first solved by Zemann & Zemann (1957). A new type of langbeinite was synthesized by replacing the SO_4 group by a BeF_4 group (Guelylah *et al.*, 1996), which exhibited several interesting low-temperature phase transitions. Langbenites are well known to exhibit ferroelectric and ferroelastic phase transitions with temperature. There are three types of langbeinites; type-I has a room-temperature cubic structure and undergoes several phase transitions to a final orthorhombic crystal form (space group $P2_12_12_1$) *via* a monoclinic crystal system (space group $P2_1$) followed by a triclinic crystal system (space group $P1$) with lowering of temperature. Type-II langbeinites show a single phase transition when cooled, resulting in an orthorhombic crystal form (space group $P2_12_12_1$). Type-III langbeinite remains invarient with lowering of temperature.

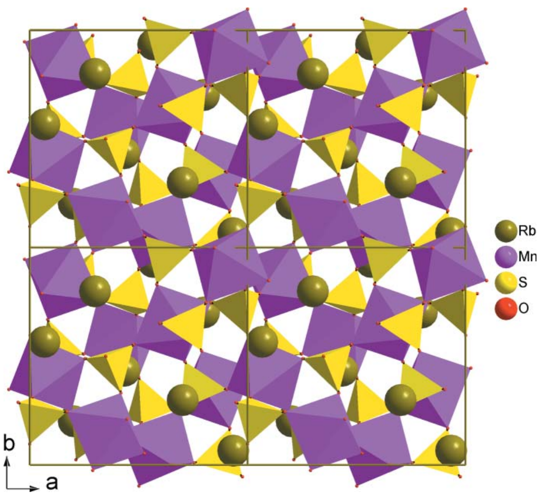

Figure 1
Packing diagram, viewed down the c axis, depicting the three-dimensional network of MnO_6 octahedra and SO_4 tetrahedra with Rb atoms in the cavities.

However, in a recent study Nalini & Guru Row (2002) have shown that $Rb_2Cd_2(SO_4)_3$ shows no intermediate triclinic form in Type-I. The title compound is isostructural with the rest of the known langbeinite family, with MnO_6 octahedra corner-shared with the SO_4 tetrahedra, as shown in Fig. 1, forming a three-dimensional network. Rb2 is nine-coordinate, whereas Rb1 is 12-coordinate, with both atoms residing in the cavities.

Experimental

The title compound was synthesized by slow evaporation at 393 K of an aqueous solution containing equimolar amounts of Rb_2SO_4 and $MnSO_4$. The evaporation rate was slowed down considerably by sealing the 5 ml beakers containing the solution in a thermostat.

Crystal data

$Rb_2Mn_2(SO_4)_3$
M_r = 569.03
Cubic, $P2_13$
a = 10.2140 (7) Å
V = 1065.58 (13) Å^3
Z = 4
D_x = 3.547 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 12.10 mm^{-1}
T = 294 (2) K
Block, colourless
0.4 × 0.2 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\rm min}$ = 0.070, $T_{\rm max}$ = 0.160
8890 measured reflections
873 independent reflections
860 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.031
$\theta_{\rm max}$ = 28.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.013
$wR(F^2)$ = 0.038
S = 1.23
873 reflections
59 parameters
$w = 1/[\sigma^2(F_o^2) + 0.4692P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max}$ = 0.001
$\Delta\rho_{\rm max}$ = 0.26 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.27 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0102 (5)
Absolute structure: Flack (1983), 339 Friedel pairs
Flack parameter: 0.013 (8)

Table 1
Selected bond lengths (Å).

Rb1—O4	2.969 (2)	Mn1—O2$^{\rm ii}$	2.176 (2)
Rb1—O2$^{\rm i}$	3.122 (2)	Mn2—O4$^{\rm vi}$	2.150 (2)
Rb1—O1	3.229 (2)	Mn2—O1$^{\rm vii}$	2.173 (2)
Rb1—O1$^{\rm ii}$	3.257 (2)	S1—O4	1.463 (2)
Rb2—O3$^{\rm iii}$	2.948 (2)	S1—O2	1.466 (2)
Rb2—O2$^{\rm iv}$	3.087 (2)	S1—O1	1.475 (2)
Rb2—O1$^{\rm iv}$	3.196 (2)	S1—O3	1.477 (2)
Mn1—O3$^{\rm v}$	2.155 (2)		

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

Data collection: *SMART* (Bruker, 2004); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *PLATON* (Spek, 2003).

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