

Dirubidium sodium manganate(V),
 $\text{Rb}_2\text{NaMnO}_4$

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Key indicators

Single-crystal X-ray study
 $T = 293 \text{ K}$
Mean $\sigma(\text{Na}-\text{O}) = 0.005 \text{ \AA}$
 R factor = 0.036
 wR factor = 0.074
Data-to-parameter ratio = 14.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

$\text{Rb}_2\text{NaMnO}_4$ has been obtained from a redox reaction in silver crucibles. The crystal structure contains isolated $[\text{MnO}_4]$ units, which are slightly distorted from ideal tetrahedral symmetry. $\text{Rb}_2\text{NaMnO}_4$ crystallizes isotypic with Cs_2NaVO_4 and $\text{Cs}_2\text{NaAsO}_4$.

Comment

$\text{Rb}_2\text{NaMnO}_4$ crystallizes isotypic with Cs_2NaVO_4 (Kissel & Hoppe, 1990) and $\text{Cs}_2\text{NaAsO}_4$ (Schneidersmann & Hoppe, 1991), but not with K_2NaMnO_4 (Fischer & Hoppe, 1992a) or $\text{Cs}_2\text{LiMnO}_4$ (Fischer & Hoppe, 1992b). The structures of the Cs_2NaMO_4 type contain the pentavalent chemical elements ($M = \text{V}, \text{Mn}, \text{As}$) in an almost tetrahedral coordination (Fig. 1). In all these cases, the discrete complex anion $[\text{MO}_4]$ is slightly distorted, with one angle $\text{O}-M-\text{O}$ close to 106° relating to the two crystallographic equivalent O atoms O3 (site 4f). These O atoms display the longest interatomic distances within the *ortho*-metallate(V) anions. The average $M-\text{O}$ distances are 1.72, 1.71 and 1.69 Å for $M = \text{V}, \text{Mn}$ and As , respectively. The coordination of the Na atoms in $\text{Rb}_2\text{NaMnO}_4$ can be described as a square pyramid of O atoms, with interatomic distances ranging from 2.262 (6) to 2.415 (4) Å. The basal O atoms connect the $[\text{NaO}_5]$ units *via trans* edges into zigzag chains along [010]. The coordination sphere of Rb1, with Rb1–O distances of 2.923 (6)–3.0560 (11) Å, corresponds to a distorted pentagonal bipyramid. These polyhedra are linked parallel to the (001) plane *via* O1, forming corrugated layers of four-membered rhomboidal entities, $[\text{Rb}_2\text{O}_1\text{O}_2]$. The second coordination sphere of Rb1, with Rb1–O3 = 3.594 (5) Å ($2\times$) has not been considered in Fig. 2, because the first coordination shell is already almost spherical within the range of the sum of the ionic radii (2.92 Å; Shannon, 1976). This is not the case for Rb2, where only four coordinating O atoms are observed in the same range of interatomic distances [2.805 (6)–3.045 (6) Å]. Along [010], these non-planar square units, $[\text{Rb}_2\text{O}_1\text{O}_2\text{O}_3]$, share *cis* edges *via* O2, leading to a double-chain arrangement. Further distances between 3.345 (4) and 3.462 (5) Å increase the coordination of Rb2 to 10 and complement the connectivity in the [100] direction of the underlying chains to the formation of layers (Fig. 2).

Experimental

$\text{Rb}_2\text{NaMnO}_4$ has been obtained from the reaction of Na_2O , Rb_2O , Mn and CdO (molar ratio 2.5:2.5:1:1) in silver crucibles, which were loaded and sealed under an argon atmosphere. For protection reasons, these containers were jacketed under vacuum in silica ampoules. The reaction mixture was heated directly to 523 K and

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then at a heating rate of 2 K h⁻¹ to 873 K. The reaction time was 14 d, then the same cooling rate was used to 523 K, after which the furnace was switched off. Green–blue single crystals of irregular shape were selected under a microscope in an argon-filled dry-box and jacketed in glass capillaries.

Crystal data

Rb₂Na(MnO₄)
M_r = 312.87
 Monoclinic, *P*2₁/*m*
a = 5.9078 (13) Å
b = 5.9821 (13) Å
c = 7.9503 (19) Å
 β = 92.22 (3)°
V = 280.76 (11) Å³
Z = 2

D_x = 3.701 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 2665 reflections
 θ = 2.6–28.1°
 μ = 19.57 mm⁻¹
T = 293 (2) K
 Irregular block, green–blue
 0.30 × 0.15 × 0.10 mm

Data collection

Stoe IPDS-I diffractometer
 φ scans
 Absorption correction: numerical
 [XRED32 (Stoe & Cie, 2001)
 XSHAPE (Stoe & Cie, 1999)]
T_{min} = 0.027, *T_{max}* = 0.086
 2023 measured reflections

670 independent reflections
 556 reflections with *I* > 2σ(*I*)
R_{int} = 0.107
 θ_{max} = 27.0°
h = -7 → 7
k = -7 → 7
l = -10 → 10

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.036
wR(*F*²) = 0.074
S = 1.01
 670 reflections
 46 parameters

$w = 1/[\sigma^2(F_o^2) + (0.0291P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δ/σ)_{max} < 0.001
 Δρ_{max} = 1.01 e Å⁻³
 Δρ_{min} = -1.51 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Rb1–O2	2.923 (6)	Rb2–O3 ⁱⁱ	3.345 (4)
Rb1–O1 ⁱ	2.966 (4)	Rb2–O3 ^{vii}	3.402 (4)
Rb1–O1	2.971 (4)	Rb2–O3 ^{viii}	3.402 (4)
Rb1–O3 ⁱⁱⁱ	2.989 (4)	Rb2–O3 ^{ix}	3.462 (5)
Rb1–O3 ⁱⁱⁱ	2.989 (4)	Rb2–O3 ^x	3.462 (5)
Rb1–O1 ⁱⁱⁱ	3.0560 (11)	Mn1–O1	1.689 (6)
Rb1–O1 ^{iv}	3.0560 (11)	Mn1–O2 ^{xi}	1.702 (5)
Rb1–O3 ^v	3.594 (5)	Mn1–O3	1.708 (3)
Rb1–O3	3.594 (5)	Mn1–O3 ^v	1.708 (3)
Rb2–O1	2.805 (6)	Na–O2	2.262 (6)
Rb2–O2 ^{iv}	3.0413 (11)	Na–O3 ^{xii}	2.316 (4)
Rb2–O2 ⁱⁱⁱ	3.0413 (11)	Na–O3 ^{xiii}	2.316 (4)
Rb2–O2 ^{vi}	3.045 (6)	Na–O3 ^v	2.415 (4)
Rb2–O3 ⁱⁱⁱ	3.345 (4)	Na–O3	2.415 (4)
O1–Mn1–O2 ^{xi}	110.8 (2)	O1–Mn1–O3 ^v	110.21 (17)
O1–Mn1–O3	110.21 (17)	O2 ^{xi} –Mn1–O3 ^v	109.86 (18)
O2 ^{xi} –Mn1–O3	109.86 (18)	O3–Mn1–O3 ^v	105.8 (2)

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

The highest peak was observed 1.04 Å from Rb2 and the deepest hole 0.68 Å from Rb1.

Data collection: *IPDS* (Stoe, 1997); cell refinement: *IPDS*; data reduction: *XRED32* (Stoe & Cie, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *CIF-Editor* (Wieczorrek, 2004).

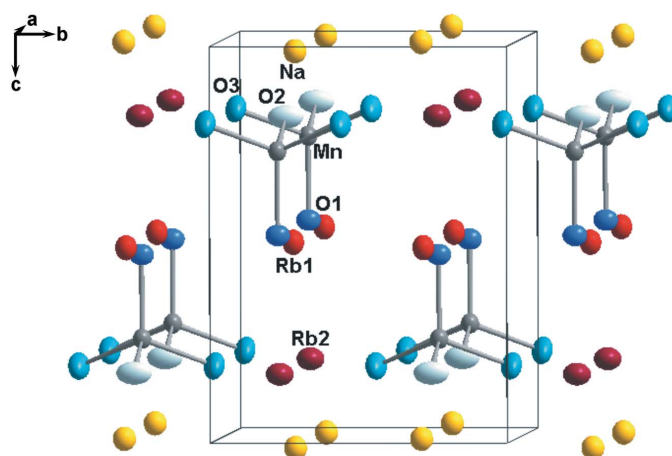


Figure 1

Perspective view of the crystal structure of Rb₂NaMnO₄, showing the atom-numbering scheme and 50% probability displacement ellipsoids.

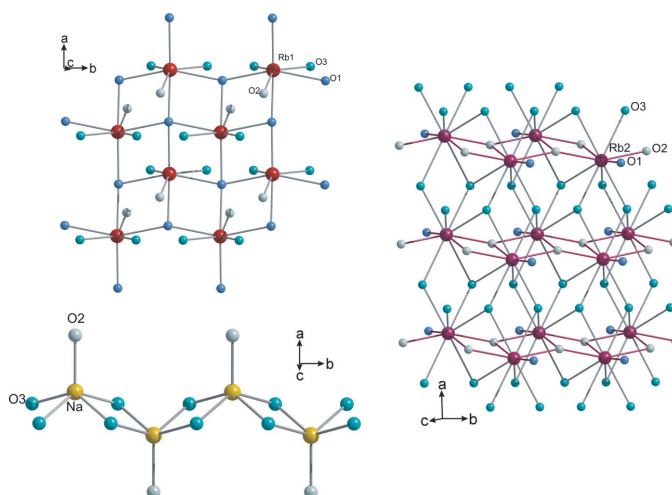


Figure 2

The coordination spheres and connectivity of Rb1, Rb2 and Na, respectively.

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