

RbSn₂(PO₄)₃, a NASICON-type phosphate

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Received 13 March 2011; accepted 16 April 2011

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{P}-\text{O}) = 0.005$ Å; R factor = 0.026; wR factor = 0.043; data-to-parameter ratio = 13.0.

The title compound, rubidium ditin(IV) tris(phosphate), RbSn₂(PO₄)₃, belongs to the NASICON-type family of phosphates and crystallizes in the space group $R\bar{3}$. The structure is composed of PO₄ tetrahedra (1 symmetry) and two slightly distorted SnO₆ octahedra, both with 3. symmetry, which are interlinked through corner-sharing O atoms to form a $\infty^3[\text{Sn}_2(\text{PO}_4)_3]^-$ framework. The Rb⁺ cations are located on threefold inversion axes in the voids of this framework and exhibit a coordination number of 12. The crystal studied was twinned by merohedry with a component ratio of 0.503:0.497.

Related literature

For related NASICON-type compounds, see: Boilot *et al.* (1987); Boujelben *et al.* (2007); Duhlev (1994); Zatovskii *et al.* (2006); Zhao *et al.* (2011).

Experimental

Crystal data

RbSn ₂ (PO ₄) ₃	$Z = 6$
$M_r = 607.76$	Mo $K\alpha$ radiation
Trigonal, $R\bar{3}$	$\mu = 10.76$ mm ⁻¹
$a = 8.340$ (4) Å	$T = 293$ K
$c = 24.007$ (8) Å	$0.20 \times 0.05 \times 0.05$ mm
$V = 1446.1$ (6) Å ³	

Data collection

Rigaku Mercury70 CCD diffractometer	3765 measured reflections
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	742 independent reflections
$T_{\min} = 0.222$, $T_{\max} = 0.615$	711 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.036$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$	57 parameters
$wR(F^2) = 0.043$	$\Delta\rho_{\text{max}} = 0.65$ e Å ⁻³
$S = 1.16$	$\Delta\rho_{\text{min}} = -0.73$ e Å ⁻³
742 reflections	

Table 1

Selected bond lengths (Å).

Sn1—O2	2.015 (4)	P1—O1	1.529 (4)
Sn1—O3 ⁱ	2.033 (4)	P1—O3	1.533 (4)
P1—O2	1.523 (4)	P1—O4	1.537 (4)

Symmetry code: (i) $y, -x + y, -z$.

Data collection: *CrystalClear* (Rigaku, 2004); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008) and *PLATON* (Spek, 2009); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2004); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

The authors acknowledge the Doctoral Foundation of Henan Polytechnic University (grant No. B2010–92, 648483).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2466).

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supplementary materials

Acta Cryst. (2011). E67, i32 [doi:10.1107/S1600536811014310]

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Comment

In recent years, the $AM_2(PO_4)_3$ (A = alkali metal; M = Ti, Zr, Ge, Sn) family with NASICON (Na₃Zr₂Si₂PO₁₂; Boilot *et al.*, 1987) -type structures attracted a growing interest due to their intriguing properties, e.g. ionic conductivity of the A cations located in the voids of the three-dimensional NASICON-type framework. This framework is composed of isolated PO₄ tetrahedra sharing corners with MO₆ octahedra (Fig. 1), and is amenable to a wide variety of chemical substitutions at the various crystallographic positions, thus yielding a large number of closely related compounds, such as NaFeNb(PO₄)₃ (Zatovskii *et al.*, 2006), Rb₂Ca₂(SO₄)₃ (Boujelben *et al.*, 2007) or Al_{0.5}Nb_{1.5}(PO₄)₃ (Zhao *et al.*, 2011). In order to augment this family of compounds, we prepared crystals of the compound RbSn₂(PO₄)₃ using a solid state reaction route. Unlike the analogous Ti compound RbTi₂(PO₄)₃ which crystallises in space group $R\bar{3}c$ (Duhlev, 1994), RbSn₂(PO₄)₃ crystallises in space group $R\bar{3}$.

A projection of the crystal structure of RbSn₂(PO₄)₃ is given in Fig. 2. It is characterized by the presence of isolated PO₄ tetrahedra (1 symmetry) and two different SnO₆ octahedra (both 3. symmetry), linked by sharing corner O atoms, to establish a three-dimensional $^3_{\infty}[\text{Sn}_2(\text{PO}_4)_3]^-$ framework. This framework delimits two types of channels in which the twelve-coordinate Rb⁺ atoms (site symmetry $\bar{3}$.) are located to compensate the negative charges. The PO₄ tetrahedra are quite regular, with P–O distances ranging from 1.523 (4) to 1.537 (4) Å. The two SnO₆ octahedra exhibit Sn—O distances ranging from 2.015 (4) to 2.033 (4) Å.

Experimental

Single crystals of RbSn₂(PO₄)₃ have been prepared by a high-temperature method in air. A powder mixture of RbNO₃, SnO₂ and NH₄H₂PO₄ in the molar ratio of Rb: Sn: P = 10: 1: 15 was first ground in an agate mortar and then transferred to a platinum crucible. The sample was gradually heated in air at 1173 K for 24 h. After that, the intermediate product was slowly cooled to 673 K at the rate of 2 K h⁻¹. It was kept at 673 K for another 10 h and then quenched to room temperature. The obtained crystals were colorless with a prismatic shape.

Refinement

The RbSn₂(PO₄)₃ crystal studies was twinned by merohedry. For refinement the twin law (0 1 0 1 0 0 0 0 T) was used; the twin component ratio refined to 0.503: 0.497. The highest peak in the difference electron density map is at a distance of 1.38 Å from Rb2 while the deepest hole is at a distance of 1.77 Å from O2.

Figures

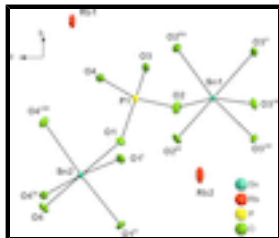


Fig. 1. The expanded asymmetric unit of $\text{RbSn}_2(\text{PO}_4)_3$ showing the coordination environments of the P and Sn atoms. The displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $-y, x-y, z$; (ii) $-x+y, -x, z$; (iii) $1-y, x-y, z$; (iv) $1-x+y, 1-x, z$; (v) $1-x, 1-y, -z$; (vi) $1+x-y, x, -z$; (vii) $y, -x+y, -z$; (Viii) $-1/3+y, 1/3-x+y, 1/3-z$; (ix) $2/3-x, 1/3-y, 1/3-z$; (x) $-1/3+x-y, -2/3+x, 1/3-z$.]

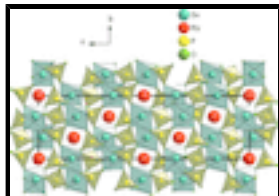


Fig. 2. View of the crystal structure of $\text{RbSn}_2(\text{PO}_4)_3$ along $[100]$. PO_4 and SnO_6 units are given in the polyhedral representation.

rubidium ditin(IV) tris(phosphate)

Crystal data

$\text{RbSn}_2(\text{PO}_4)_3$

$M_r = 607.76$

Trigonal, $R\bar{3}$

Hall symbol: $-R\ 3$

$a = 8.340$ (4) Å

$c = 24.007$ (8) Å

$V = 1446.1$ (6) Å³

$Z = 6$

$F(000) = 1668$

$D_x = 4.187$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1316 reflections

$\theta = 2.6\text{--}27.5^\circ$

$\mu = 10.76$ mm⁻¹

$T = 293$ K

Prism, colourless

$0.20 \times 0.05 \times 0.05$ mm

Data collection

Rigaku Mercury70 CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 14.6306 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.222$, $T_{\max} = 0.615$

3765 measured reflections

742 independent reflections

711 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.6^\circ$

$h = -9 \rightarrow 10$

$k = -10 \rightarrow 10$

$l = -29 \rightarrow 31$

Refinement

Refinement on F^2

Least-squares matrix: full

0 restraints

Primary atom site location: structure-invariant direct
methods

$$R[F^2 > 2\sigma(F^2)] = 0.026$$

$$wR(F^2) = 0.043$$

$$S = 1.16$$

742 reflections

57 parameters

Secondary atom site location: difference Fourier map

$$w = 1/[\sigma^2(F_o^2) + (0.0097P)^2 + 13.5872P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$\Delta\rho_{\max} = 0.65 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.73 \text{ e } \text{\AA}^{-3}$$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn1	0.6667	0.3333	-0.01707 (2)	0.00467 (15)
Rb1	0.3333	0.6667	0.1667	0.0164 (3)
P1	0.3780 (2)	0.3319 (3)	0.08383 (7)	0.0058 (2)
O1	0.2172 (6)	0.1463 (5)	0.10332 (14)	0.0090 (9)
Sn2	0.0000	0.0000	0.15528 (2)	0.00490 (15)
Rb2	0.0000	0.0000	0.0000	0.0227 (4)
O2	0.4497 (6)	0.2928 (6)	0.03015 (16)	0.0119 (10)
O3	0.3083 (6)	0.4664 (6)	0.07059 (16)	0.0093 (9)
O4	0.5248 (6)	0.4207 (6)	0.12987 (14)	0.0103 (10)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0051 (2)	0.0051 (2)	0.0039 (3)	0.00253 (11)	0.000	0.000
Rb1	0.0221 (5)	0.0221 (5)	0.0051 (5)	0.0111 (2)	0.000	0.000
P1	0.0046 (8)	0.0068 (6)	0.0050 (6)	0.0022 (7)	0.0000 (6)	0.0008 (5)
O1	0.008 (2)	0.008 (2)	0.0097 (17)	0.0028 (17)	0.0044 (15)	0.0025 (14)
Sn2	0.0055 (2)	0.0055 (2)	0.0037 (3)	0.00275 (11)	0.000	0.000
Rb2	0.0304 (6)	0.0304 (6)	0.0073 (6)	0.0152 (3)	0.000	0.000
O2	0.009 (2)	0.018 (2)	0.009 (2)	0.008 (2)	0.0020 (17)	-0.0029 (17)
O3	0.014 (2)	0.010 (2)	0.0064 (17)	0.0077 (19)	-0.0023 (16)	0.0001 (16)
O4	0.011 (2)	0.008 (2)	0.0100 (17)	0.003 (2)	-0.0050 (17)	-0.0005 (16)

supplementary materials

Geometric parameters (Å, °)

Sn1—O2 ⁱ	2.015 (4)	P1—Rb2	3.595 (2)
Sn1—O2 ⁱⁱ	2.015 (4)	O1—Sn2	2.029 (4)
Sn1—O2	2.015 (4)	O1—Rb2	2.952 (4)
Sn1—O3 ⁱⁱⁱ	2.033 (4)	Sn2—O1 ^{xii}	2.029 (4)
Sn1—O3 ^{iv}	2.033 (4)	Sn2—O1 ^{xiii}	2.029 (4)
Sn1—O3 ^v	2.033 (4)	Sn2—O4 ^{xiv}	2.033 (4)
Sn1—Rb1 ^{vi}	3.5915 (13)	Sn2—O4 ^{xv}	2.033 (4)
Rb1—O3 ^{vii}	2.794 (4)	Sn2—O4 ^{viii}	2.033 (4)
Rb1—O3 ^{viii}	2.794 (4)	Sn2—Rb2	3.7278 (13)
Rb1—O3 ^{ix}	2.794 (4)	Rb2—O1 ^{xvi}	2.952 (4)
Rb1—O3	2.793 (4)	Rb2—O1 ^{xii}	2.952 (4)
Rb1—O3 ^x	2.794 (4)	Rb2—O1 ^{xvii}	2.952 (4)
Rb1—O3 ^{xi}	2.794 (4)	Rb2—O1 ^{iv}	2.952 (4)
Rb1—O4 ^{vii}	3.289 (5)	Rb2—O1 ^{xiii}	2.952 (4)
Rb1—O4 ^x	3.288 (5)	Rb2—O2 ^{xvii}	3.375 (5)
Rb1—O4 ^{ix}	3.288 (5)	Rb2—O2 ^{xvi}	3.375 (5)
Rb1—O4 ^{viii}	3.288 (5)	Rb2—O2 ^{xii}	3.375 (5)
Rb1—O4 ^{xi}	3.288 (5)	Rb2—O2 ^{iv}	3.375 (5)
Rb1—O4	3.288 (5)	Rb2—O2 ^{xiii}	3.375 (5)
P1—O2	1.523 (4)	Rb2—O2	3.376 (5)
P1—O1	1.529 (4)	O3—Sn1 ^v	2.034 (4)
P1—O3	1.533 (4)	O4—Sn2 ^{xiv}	2.033 (4)
P1—O4	1.537 (4)		
O2 ⁱ —Sn1—O2 ⁱⁱ	91.47 (17)	Rb2—P1—Rb1	121.07 (4)
O2 ⁱ —Sn1—O2	91.47 (17)	P1—O1—Sn2	149.8 (3)
O2 ⁱⁱ —Sn1—O2	91.47 (17)	P1—O1—Rb2	101.98 (17)
O2 ⁱ —Sn1—O3 ⁱⁱⁱ	83.62 (17)	Sn2—O1—Rb2	95.11 (15)
O2 ⁱⁱ —Sn1—O3 ⁱⁱⁱ	102.00 (17)	O1—Sn2—O1 ^{xii}	86.16 (16)
O2—Sn1—O3 ⁱⁱⁱ	165.74 (17)	O1—Sn2—O1 ^{xiii}	86.16 (16)
O2 ⁱ —Sn1—O3 ^{iv}	102.00 (17)	O1 ^{xii} —Sn2—O1 ^{xiii}	86.16 (16)
O2 ⁱⁱ —Sn1—O3 ^{iv}	165.74 (17)	O1—Sn2—O4 ^{xiv}	93.48 (16)
O2—Sn1—O3 ^{iv}	83.62 (17)	O1 ^{xii} —Sn2—O4 ^{xiv}	89.54 (16)
O3 ⁱⁱⁱ —Sn1—O3 ^{iv}	84.32 (17)	O1 ^{xiii} —Sn2—O4 ^{xiv}	175.70 (16)
O2 ⁱ —Sn1—O3 ^v	165.74 (17)	O1—Sn2—O4 ^{xv}	175.70 (16)
O2 ⁱⁱ —Sn1—O3 ^v	83.62 (17)	O1 ^{xii} —Sn2—O4 ^{xv}	93.48 (16)
O2—Sn1—O3 ^v	102.00 (17)	O1 ^{xiii} —Sn2—O4 ^{xv}	89.54 (16)
O3 ⁱⁱⁱ —Sn1—O3 ^v	84.32 (17)	O4 ^{xiv} —Sn2—O4 ^{xv}	90.80 (16)
O3 ^{iv} —Sn1—O3 ^v	84.32 (17)	O1—Sn2—O4 ^{viii}	89.54 (16)
O2 ⁱ —Sn1—Rb1 ^{vi}	124.22 (12)	O1 ^{xii} —Sn2—O4 ^{viii}	175.70 (16)

O2 ⁱⁱ —Sn1—Rb1 ^{vi}	124.22 (12)	O1 ^{xiii} —Sn2—O4 ^{viii}	93.48 (16)
O2—Sn1—Rb1 ^{vi}	124.22 (12)	O4 ^{xiv} —Sn2—O4 ^{viii}	90.80 (16)
O3 ⁱⁱⁱ —Sn1—Rb1 ^{vi}	50.81 (11)	O4 ^{xv} —Sn2—O4 ^{viii}	90.80 (16)
O3 ^{iv} —Sn1—Rb1 ^{vi}	50.81 (11)	O1—Sn2—Rb2	52.06 (11)
O3 ^v —Sn1—Rb1 ^{vi}	50.81 (11)	O1 ^{xii} —Sn2—Rb2	52.06 (11)
O3 ^{vii} —Rb1—O3 ^{viii}	58.49 (13)	O1 ^{xiii} —Sn2—Rb2	52.06 (11)
O3 ^{vii} —Rb1—O3 ^{ix}	58.49 (13)	O4 ^{xiv} —Sn2—Rb2	124.70 (11)
O3 ^{viii} —Rb1—O3 ^{ix}	58.49 (13)	O4 ^{xv} —Sn2—Rb2	124.69 (11)
O3 ^{vii} —Rb1—O3	180.0	O4 ^{viii} —Sn2—Rb2	124.69 (11)
O3 ^{viii} —Rb1—O3	121.51 (13)	O1 ^{xvi} —Rb2—O1 ^{xii}	180.0 (3)
O3 ^{ix} —Rb1—O3	121.51 (13)	O1 ^{xvi} —Rb2—O1 ^{xvii}	56.00 (13)
O3 ^{vii} —Rb1—O3 ^x	121.51 (13)	O1 ^{xii} —Rb2—O1 ^{xvii}	124.00 (13)
O3 ^{viii} —Rb1—O3 ^x	121.51 (13)	O1 ^{xvi} —Rb2—O1 ^{iv}	56.00 (13)
O3 ^{ix} —Rb1—O3 ^x	180.0	O1 ^{xii} —Rb2—O1 ^{iv}	124.00 (13)
O3—Rb1—O3 ^x	58.49 (13)	O1 ^{xvii} —Rb2—O1 ^{iv}	56.00 (13)
O3 ^{vii} —Rb1—O3 ^{xi}	121.51 (13)	O1 ^{xvi} —Rb2—O1 ^{xiii}	124.00 (13)
O3 ^{viii} —Rb1—O3 ^{xi}	180.0	O1 ^{xii} —Rb2—O1 ^{xiii}	56.00 (13)
O3 ^{ix} —Rb1—O3 ^{xi}	121.51 (13)	O1 ^{xvii} —Rb2—O1 ^{xiii}	124.00 (13)
O3—Rb1—O3 ^{xi}	58.49 (13)	O1 ^{iv} —Rb2—O1 ^{xiii}	180.00 (17)
O3 ^x —Rb1—O3 ^{xi}	58.49 (13)	O1 ^{xvi} —Rb2—O1	124.00 (13)
O3 ^{vii} —Rb1—O4 ^{vii}	47.14 (10)	O1 ^{xii} —Rb2—O1	56.00 (13)
O3 ^{viii} —Rb1—O4 ^{vii}	75.80 (10)	O1 ^{xvii} —Rb2—O1	180.0
O3 ^{ix} —Rb1—O4 ^{vii}	105.07 (10)	O1 ^{iv} —Rb2—O1	124.00 (13)
O3—Rb1—O4 ^{vii}	132.87 (10)	O1 ^{xiii} —Rb2—O1	56.00 (13)
O3 ^x —Rb1—O4 ^{vii}	74.93 (10)	O1 ^{xvi} —Rb2—O2 ^{xvii}	94.20 (11)
O3 ^{xi} —Rb1—O4 ^{vii}	104.20 (10)	O1 ^{xii} —Rb2—O2 ^{xvii}	85.80 (11)
O3 ^{vii} —Rb1—O4 ^x	104.20 (11)	O1 ^{xvii} —Rb2—O2 ^{xvii}	44.81 (10)
O3 ^{viii} —Rb1—O4 ^x	74.93 (10)	O1 ^{iv} —Rb2—O2 ^{xvii}	95.50 (10)
O3 ^{ix} —Rb1—O4 ^x	132.86 (10)	O1 ^{xiii} —Rb2—O2 ^{xvii}	84.50 (10)
O3—Rb1—O4 ^x	75.80 (11)	O1—Rb2—O2 ^{xvii}	135.19 (10)
O3 ^x —Rb1—O4 ^x	47.14 (10)	O1 ^{xvi} —Rb2—O2 ^{xvi}	44.81 (10)
O3 ^{xi} —Rb1—O4 ^x	105.07 (10)	O1 ^{xii} —Rb2—O2 ^{xvi}	135.19 (10)
O4 ^{vii} —Rb1—O4 ^x	66.94 (5)	O1 ^{xvii} —Rb2—O2 ^{xvi}	95.50 (10)
O3 ^{vii} —Rb1—O4 ^{ix}	75.80 (11)	O1 ^{iv} —Rb2—O2 ^{xvi}	94.20 (11)
O3 ^{viii} —Rb1—O4 ^{ix}	105.07 (10)	O1 ^{xiii} —Rb2—O2 ^{xvi}	85.80 (11)
O3 ^{ix} —Rb1—O4 ^{ix}	47.14 (10)	O1—Rb2—O2 ^{xvi}	84.50 (10)
O3—Rb1—O4 ^{ix}	104.20 (11)	O2 ^{xvii} —Rb2—O2 ^{xvi}	115.54 (5)
O3 ^x —Rb1—O4 ^{ix}	132.87 (10)	O1 ^{xvi} —Rb2—O2 ^{xii}	135.19 (10)
O3 ^{xi} —Rb1—O4 ^{ix}	74.93 (10)	O1 ^{xii} —Rb2—O2 ^{xii}	44.81 (10)
O4 ^{vii} —Rb1—O4 ^{ix}	113.06 (5)	O1 ^{xvii} —Rb2—O2 ^{xii}	84.50 (10)
O4 ^x —Rb1—O4 ^{ix}	180.0	O1 ^{iv} —Rb2—O2 ^{xii}	85.80 (11)

supplementary materials

O3 ^{vii} —Rb1—O4 ^{viii}	105.07 (10)	O1 ^{xiii} —Rb2—O2 ^{xii}	94.20 (11)
O3 ^{viii} —Rb1—O4 ^{viii}	47.14 (10)	O1—Rb2—O2 ^{xii}	95.50 (10)
O3 ^{ix} —Rb1—O4 ^{viii}	75.80 (11)	O2 ^{xvii} —Rb2—O2 ^{xii}	64.46 (5)
O3—Rb1—O4 ^{viii}	74.93 (10)	O2 ^{xvi} —Rb2—O2 ^{xii}	180.00 (19)
O3 ^x —Rb1—O4 ^{viii}	104.20 (11)	O1 ^{xvi} —Rb2—O2 ^{iv}	95.50 (10)
O3 ^{xi} —Rb1—O4 ^{viii}	132.87 (10)	O1 ^{xii} —Rb2—O2 ^{iv}	84.50 (10)
O4 ^{vii} —Rb1—O4 ^{viii}	113.06 (5)	O1 ^{xvii} —Rb2—O2 ^{iv}	94.20 (11)
O4 ^x —Rb1—O4 ^{viii}	66.94 (5)	O1 ^{iv} —Rb2—O2 ^{iv}	44.81 (10)
O4 ^{ix} —Rb1—O4 ^{viii}	113.06 (5)	O1 ^{xiii} —Rb2—O2 ^{iv}	135.19 (10)
O3 ^{vii} —Rb1—O4 ^{xi}	74.93 (10)	O1—Rb2—O2 ^{iv}	85.80 (11)
O3 ^{viii} —Rb1—O4 ^{xi}	132.86 (10)	O2 ^{xvii} —Rb2—O2 ^{iv}	115.54 (5)
O3 ^{ix} —Rb1—O4 ^{xi}	104.20 (11)	O2 ^{xvi} —Rb2—O2 ^{iv}	115.54 (5)
O3—Rb1—O4 ^{xi}	105.08 (10)	O2 ^{xii} —Rb2—O2 ^{iv}	64.46 (5)
O3 ^x —Rb1—O4 ^{xi}	75.80 (11)	O1 ^{xvi} —Rb2—O2 ^{xiii}	84.50 (10)
O3 ^{xi} —Rb1—O4 ^{xi}	47.14 (10)	O1 ^{xii} —Rb2—O2 ^{xiii}	95.50 (10)
O4 ^{vii} —Rb1—O4 ^{xi}	66.94 (5)	O1 ^{xvii} —Rb2—O2 ^{xiii}	85.80 (11)
O4 ^x —Rb1—O4 ^{xi}	113.06 (5)	O1 ^{iv} —Rb2—O2 ^{xiii}	135.19 (10)
O4 ^{ix} —Rb1—O4 ^{xi}	66.94 (5)	O1 ^{xiii} —Rb2—O2 ^{xiii}	44.81 (10)
O4 ^{viii} —Rb1—O4 ^{xi}	180.0	O1—Rb2—O2 ^{xiii}	94.20 (11)
O3 ^{vii} —Rb1—O4	132.86 (10)	O2 ^{xvii} —Rb2—O2 ^{xiii}	64.46 (5)
O3 ^{viii} —Rb1—O4	104.20 (10)	O2 ^{xvi} —Rb2—O2 ^{xiii}	64.46 (5)
O3 ^{ix} —Rb1—O4	74.92 (10)	O2 ^{xii} —Rb2—O2 ^{xiii}	115.54 (5)
O3—Rb1—O4	47.14 (10)	O2 ^{iv} —Rb2—O2 ^{xiii}	180.0 (2)
O3 ^x —Rb1—O4	105.08 (10)	O1 ^{xvi} —Rb2—O2	85.80 (11)
O3 ^{xi} —Rb1—O4	75.80 (10)	O1 ^{xii} —Rb2—O2	94.20 (11)
O4 ^{vii} —Rb1—O4	180.0	O1 ^{xvii} —Rb2—O2	135.19 (10)
O4 ^x —Rb1—O4	113.06 (5)	O1 ^{iv} —Rb2—O2	84.50 (10)
O4 ^{ix} —Rb1—O4	66.94 (5)	O1 ^{xiii} —Rb2—O2	95.50 (10)
O4 ^{viii} —Rb1—O4	66.94 (5)	O1—Rb2—O2	44.81 (10)
O4 ^{xi} —Rb1—O4	113.06 (5)	O2 ^{xvii} —Rb2—O2	180.0
O2—P1—O1	106.4 (3)	O2 ^{xvi} —Rb2—O2	64.47 (5)
O2—P1—O3	108.3 (2)	O2 ^{xii} —Rb2—O2	115.53 (5)
O1—P1—O3	110.1 (3)	O2 ^{iv} —Rb2—O2	64.46 (5)
O2—P1—O4	114.1 (2)	O2 ^{xiii} —Rb2—O2	115.54 (5)
O1—P1—O4	110.6 (2)	P1—O2—Sn1	148.8 (3)
O3—P1—O4	107.4 (2)	P1—O2—Rb2	85.6 (2)
O2—P1—Rb2	69.43 (19)	Sn1—O2—Rb2	125.48 (17)
O1—P1—Rb2	53.44 (15)	P1—O3—Sn1 ^v	144.2 (3)
O3—P1—Rb2	86.57 (16)	P1—O3—Rb1	108.91 (19)
O4—P1—Rb2	162.60 (19)	Sn1 ^v —O3—Rb1	94.85 (15)
O2—P1—Rb1	147.0 (2)	P1—O4—Sn2 ^{xiv}	134.6 (3)

O1—P1—Rb1	103.79 (16)	P1—O4—Rb1	88.59 (19)
O3—P1—Rb1	47.30 (15)	Sn2 ^{xiv} —O4—Rb1	128.46 (15)
O4—P1—Rb1	66.10 (17)		

Symmetry codes: (i) $-y+1, x-y, z$; (ii) $-x+y+1, -x+1, z$; (iii) $x-y+1, x, -z$; (iv) $y, -x+y, -z$; (v) $-x+1, -y+1, -z$; (vi) $x+1/3, y-1/3, z-1/3$; (vii) $-x+2/3, -y+4/3, -z+1/3$; (viii) $y-1/3, -x+y+1/3, -z+1/3$; (ix) $x-y+2/3, x+1/3, -z+1/3$; (x) $-x+y, -x+1, z$; (xi) $-y+1, x-y+1, z$; (xii) $-x+y, -x, z$; (xiii) $-y, x-y, z$; (xiv) $-x+2/3, -y+1/3, -z+1/3$; (xv) $x-y-1/3, x-2/3, -z+1/3$; (xvi) $x-y, x, -z$; (xvii) $-x, -y, -z$.

Fig. 1

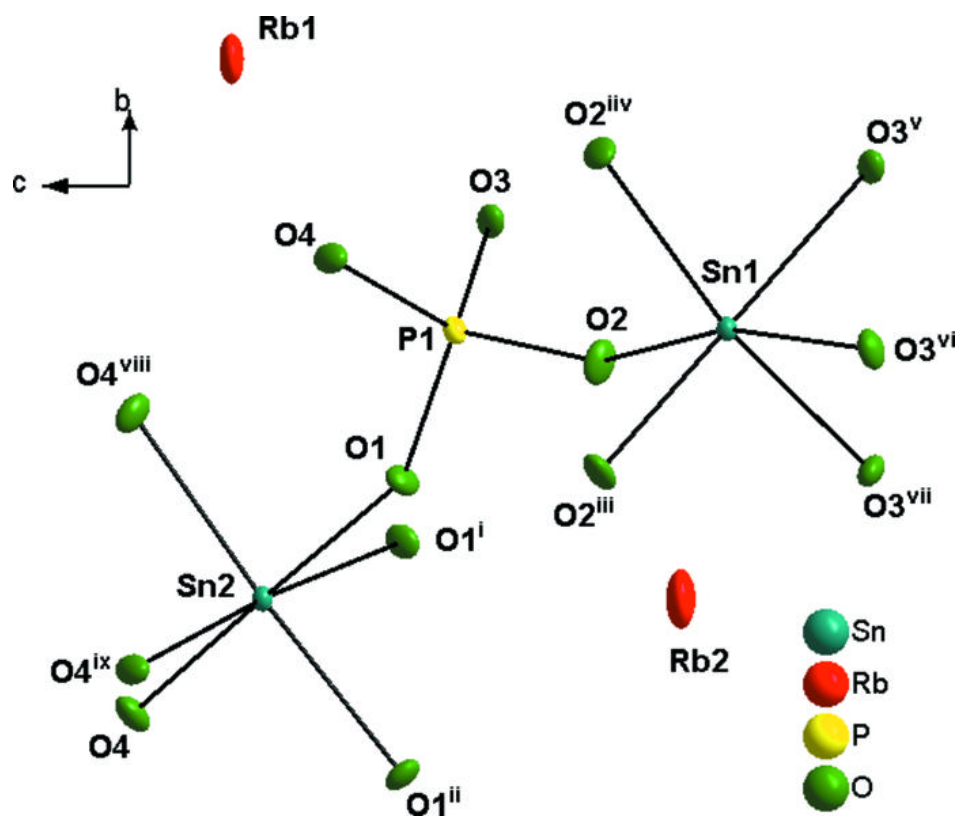


Fig. 2

