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Potassium ditin(IV) tris[phosphate(V)],
KSn₂(PO₄)₃

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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{Sn}-\text{O}) = 0.008$ Å;
 R factor = 0.053; wR factor = 0.137; data-to-parameter ratio = 10.3.

The title compound, KSn₂(PO₄)₃, belongs to the NASICON-type family of phosphates with the space group $R\bar{3}$. Its structure is constructed by very regular [with P—O distances ranging from 1.513 (6) to 1.522 (6) Å] PO₄ tetrahedra and SnO₆ octahedra on the 3. axis, which are linked by O atoms, forming an [Sn₂(PO₄)₃] framework. The K atoms occupy the $\bar{3}$. axis sites and are located in the voids of this arrangement. The crystal studied was a merohedral twin with twin law (010 100 00 $\bar{1}$) and a component ratio of 0.580 (7):0.420 (7).

Related literature

For related NASICON-type compounds, see: Alamo & Rodrigo (1992); Boilot *et al.* (1987); Boujelben *et al.* (2007); Zatonvskii *et al.* (2006); Zhao *et al.* (2011).

Experimental

Crystal data

KSn₂(PO₄)₃ $Z = 6$
 $M_r = 561.39$ Mo $K\alpha$ radiation
 Trigonal, $R\bar{3}$ $\mu = 6.30$ mm⁻¹
 $a = 8.3381$ (1) Å $T = 296$ K
 $c = 23.5508$ (3) Å $0.20 \times 0.05 \times 0.05$ mm
 $V = 1417.98$ (3) Å³

Data collection

Bruker SMART 1K CCD 2168 measured reflections
 diffractometer 597 independent reflections
 Absorption correction: multi-scan 591 reflections with $I > 2\sigma(I)$
 (SADABS; Bruker, 1997) $R_{\text{int}} = 0.098$
 $T_{\text{min}} = 0.366$, $T_{\text{max}} = 0.744$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$ 58 parameters
 $wR(F^2) = 0.137$ $\Delta\rho_{\text{max}} = 2.23$ e Å⁻³
 $S = 1.24$ $\Delta\rho_{\text{min}} = -2.99$ e Å⁻³
 597 reflections

Data collection: SMART (Bruker, 1997); cell refinement: SMART; data reduction: SAINT (Bruker, 1997); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 2004); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2111).

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supplementary materials

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Potassium ditin(IV) tris[phosphate(V)], $\text{KSn}_2(\text{PO}_4)_3$

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Comment

In the past, the family of $AM_2(\text{PO}_4)_3$ (A = alkali metals; M = Ti, Zr, Ge, Sn) compounds with the NASICON-type ($\text{Na}_3\text{Zr}_2\text{Si}_2\text{PO}_{12}$; Boilot, *et al.*, 1987) structure have been extensively investigated for their intriguing properties, such as the ionic conductivity properties which may due to the complex and subtle interactions between NASICON framework and mobile ions. The NASICON-type structure with a flexible three-dimensional framework of PO_4 tetrahedra sharing corners with MO_6 octahedra, 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 $\text{NaFeNb}(\text{PO}_4)_3$ (Zatovskii, *et al.*, 2006) and $\text{K}_2\text{Ca}_2(\text{SO}_4)_3$ (Boujelben, *et al.*, 2007). In order to enrich this family of compounds, we synthesis the compound $\text{KSn}_2(\text{PO}_4)_3$ by the high-temperature reaction and determine the crystal structure from single-crystal X-ray diffraction analysis. $\text{KSn}_2(\text{PO}_4)_3$ is isostructure with Na (Alamo & Rodrigo, 1992) and Rb (Zhao *et al.*, 2011) analog crystals which crystallizes in the trigonal space group $R\bar{3}$.

A projection of the crystal structure of $\text{KSn}_2(\text{PO}_4)_3$ is given in Fig. 2. It is characterized by the presence of PO_4 tetrahedra and SnO_6 octahedra, linked by sharing corner O atoms, to establish a three-dimensional $[\text{Sn}_2(\text{PO}_4)_3]$ framework. Furthermore, this framework delimits two types of channels in which the K atoms are located to compensate the negative charges. The PO_4 tetrahedra are quite regular, with the P–O distance ranging from 1.513 (6) to 1.522 (6) Å, while the SnO_6 octahedra is quite regular too, with the Sn–O distance ranging from 2.003 (6) to 2.045 (6) Å.

Experimental

Compound $\text{KSn}_2(\text{PO}_4)_3$ has been prepared by a high-temperature method in air. A powder mixture of K_2CO_3 , SnO_2 and $\text{NH}_4\text{H}_2\text{PO}_4$ in the molar ratio of K: Sn: P = 15: 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 773 K at the rate of 2 K h^{-1} , and finally quenched to room temperature. The obtained crystals were colorless with a prismatic shape.

Refinement

The $\text{KSn}_2(\text{PO}_4)_3$ crystal studies was twinned by merohedry. For refinement the twin law (0 1 0 1 0 0 0 1) was used; the twin component ratio refined to 0.580 (7): 0.420 (7). The highest peak in the difference electron density map equals to $2.23 \text{ e}/\text{\AA}^3$ at the distance of 0.05 Å from Sn1 site while the deepest hole equals to $-2.99 \text{ e}/\text{\AA}^3$ at the distance of 0.99 Å from Sn2 site.

Figures

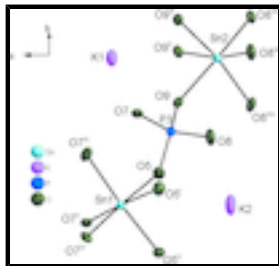


Fig. 1. The expanded asymmetric unit of $\text{KSn}_2(\text{PO}_4)_3$ showing the coordination environments of the P and Sn atoms. The displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $-x + y, -x, z$; (ii) $-y, x - y, z$; (iii) $y - 1/3, -x + y - 2/3, -z + 1/3$; (v)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

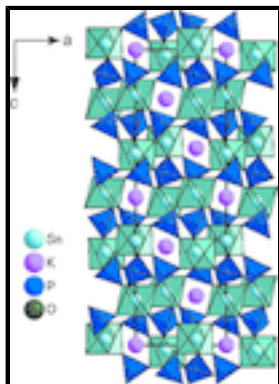


Fig. 2. View of the crystal structure of $\text{KSn}_2(\text{PO}_4)_3$ along $[010]$. PO_4 and SnO_6 units are given in the polyhedral representation.

Potassium ditin(IV) tris[phosphate(V)]

Crystal data

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

$M_r = 561.39$

Trigonal, $R\bar{3}$

Hall symbol: $-R\ 3$

$a = 8.3381(1)\ \text{\AA}$

$c = 23.5508(3)\ \text{\AA}$

$V = 1417.98(3)\ \text{\AA}^3$

$Z = 6$

$F(000) = 1560$

$D_x = 3.945\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 256 reflections

$\theta = 2.6\text{--}23.6^\circ$

$\mu = 6.30\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Prism, colourless

$0.20 \times 0.05 \times 0.05\ \text{mm}$

Data collection

Bruker SMART 1K CCD
diffractometer

Radiation source: fine-focus sealed tube
graphite

\ scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 1997)

$T_{\min} = 0.366, T_{\max} = 0.744$

2168 measured reflections

597 independent reflections

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

$R_{\text{int}} = 0.098$

$\theta_{\text{max}} = 25.7^\circ, \theta_{\text{min}} = 3.0^\circ$

$h = -10 \rightarrow 10$

$k = -10 \rightarrow 10$

$l = -17 \rightarrow 28$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.053$	$w = 1/[\sigma^2(F_o^2) + (0.0764P)^2 + 11.5796P]$
$wR(F^2) = 0.137$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.24$	$(\Delta/\sigma)_{\max} < 0.001$
597 reflections	$\Delta\rho_{\max} = 2.23 \text{ e } \text{\AA}^{-3}$
58 parameters	$\Delta\rho_{\min} = -2.99 \text{ e } \text{\AA}^{-3}$
0 restraints	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.0063 (7)

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	0.0000	0.0000	0.15357 (4)	0.0107 (5)
Sn2	0.3333	0.6667	0.01858 (4)	0.0103 (5)
K1	0.3333	0.6667	0.1667	0.0273 (12)
K2	0.0000	0.0000	0.0000	0.0378 (14)
P3	-0.0441 (3)	0.3326 (4)	0.08384 (9)	0.0117 (6)
O5	-0.0732 (11)	0.1435 (9)	0.1006 (2)	0.0174 (15)
O7	-0.1043 (9)	0.4149 (9)	0.1310 (2)	0.0154 (14)
O8	-0.1477 (9)	0.3069 (10)	0.0284 (3)	0.0208 (15)
O9	0.1599 (8)	0.4650 (8)	0.0738 (2)	0.0140 (15)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0111 (6)	0.0111 (6)	0.0099 (6)	0.0056 (3)	0.000	0.000
Sn2	0.0108 (5)	0.0108 (5)	0.0093 (6)	0.0054 (3)	0.000	0.000
K1	0.0332 (17)	0.0332 (17)	0.015 (2)	0.0166 (9)	0.000	0.000
K2	0.050 (2)	0.050 (2)	0.014 (2)	0.0248 (11)	0.000	0.000
P3	0.0115 (12)	0.0118 (11)	0.0109 (11)	0.0052 (9)	0.0006 (9)	0.0003 (9)

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O5	0.024 (4)	0.018 (4)	0.017 (3)	0.015 (3)	0.001 (3)	0.001 (2)
O7	0.023 (3)	0.009 (3)	0.016 (3)	0.009 (3)	0.006 (3)	0.000 (3)
O8	0.020 (4)	0.032 (4)	0.011 (3)	0.013 (3)	-0.003 (3)	0.002 (3)
O9	0.016 (3)	0.014 (3)	0.012 (3)	0.006 (3)	0.000 (2)	-0.003 (2)

Geometric parameters (\AA , $^\circ$)

Sn1—O5 ⁱ	2.023 (6)	K1—O7 ^{iv}	3.282 (7)
Sn1—O5 ⁱⁱ	2.023 (6)	K1—O7 ^{xii}	3.282 (7)
Sn1—O5	2.023 (6)	K1—O7 ^{xi}	3.282 (7)
Sn1—O7 ⁱⁱⁱ	2.032 (6)	K1—O7 ^x	3.282 (7)
Sn1—O7 ^{iv}	2.033 (6)	K2—O5	2.853 (6)
Sn1—O7 ^v	2.033 (6)	K2—O5 ^{xiii}	2.854 (6)
Sn1—K2	3.6167 (9)	K2—O5 ⁱ	2.854 (6)
Sn2—O8 ^{vi}	2.003 (6)	K2—O5 ^{viii}	2.854 (6)
Sn2—O8 ^{vii}	2.003 (6)	K2—O5 ⁱⁱ	2.854 (6)
Sn2—O8 ^{viii}	2.003 (6)	K2—O5 ^{xiv}	2.854 (6)
Sn2—O9 ^{ix}	2.045 (6)	K2—O8 ^{xiii}	3.416 (7)
Sn2—O9	2.045 (6)	K2—O8 ⁱ	3.416 (7)
Sn2—O9 ^x	2.045 (6)	K2—O8 ^{viii}	3.416 (7)
Sn2—K1	3.4876 (9)	K2—O8 ⁱⁱ	3.416 (7)
K1—O9 ^{xi}	2.696 (6)	K2—O8 ^{xiv}	3.416 (7)
K1—O9 ^{xii}	2.696 (6)	K2—O8	3.416 (7)
K1—O9 ^{iv}	2.696 (6)	P3—O9	1.513 (6)
K1—O9 ^{ix}	2.696 (6)	P3—O7	1.516 (6)
K1—O9	2.696 (6)	P3—O8	1.520 (6)
K1—O9 ^x	2.696 (6)	P3—O5	1.522 (6)
K1—O7 ^{ix}	3.282 (7)	O7—Sn1 ^v	2.033 (6)
K1—O7	3.282 (7)	O8—Sn2 ^{vi}	2.003 (6)
O5 ⁱ —Sn1—O5 ⁱⁱ	85.9 (2)	O9—K1—O7 ^x	76.59 (17)
O5 ⁱ —Sn1—O5	85.9 (2)	O9 ^x —K1—O7 ^x	46.76 (15)
O5 ⁱⁱ —Sn1—O5	85.9 (2)	O7 ^{ix} —K1—O7 ^x	113.67 (8)
O5 ⁱ —Sn1—O7 ⁱⁱⁱ	90.7 (2)	O7—K1—O7 ^x	113.67 (8)
O5 ⁱⁱ —Sn1—O7 ⁱⁱⁱ	92.1 (2)	O7 ^{iv} —K1—O7 ^x	66.33 (8)
O5—Sn1—O7 ⁱⁱⁱ	176.2 (2)	O7 ^{xii} —K1—O7 ^x	66.33 (8)
O5 ⁱ —Sn1—O7 ^{iv}	92.1 (2)	O7 ^{xi} —K1—O7 ^x	180.00 (14)
O5 ⁱⁱ —Sn1—O7 ^{iv}	176.2 (2)	O5—K2—O5 ^{xiii}	122.2 (2)
O5—Sn1—O7 ^{iv}	90.7 (2)	O5—K2—O5 ⁱ	57.8 (2)
O7 ⁱⁱⁱ —Sn1—O7 ^{iv}	91.2 (2)	O5 ^{xiii} —K2—O5 ⁱ	180.0 (6)
O5 ⁱ —Sn1—O7 ^v	176.2 (2)	O5—K2—O5 ^{viii}	122.2 (2)
O5 ⁱⁱ —Sn1—O7 ^v	90.7 (2)	O5 ^{xiii} —K2—O5 ^{viii}	57.8 (2)
O5—Sn1—O7 ^v	92.1 (2)	O5 ⁱ —K2—O5 ^{viii}	122.2 (2)

O7 ⁱⁱⁱ —Sn1—O7 ^v	91.2 (2)	O5—K2—O5 ⁱⁱ	57.8 (2)
O7 ^{iv} —Sn1—O7 ^v	91.2 (2)	O5 ^{xiii} —K2—O5 ⁱⁱ	122.2 (2)
O5 ⁱ —Sn1—K2	51.89 (17)	O5 ⁱ —K2—O5 ⁱⁱ	57.8 (2)
O5 ⁱⁱ —Sn1—K2	51.89 (17)	O5 ^{viii} —K2—O5 ⁱⁱ	180.0 (3)
O5—Sn1—K2	51.89 (17)	O5—K2—O5 ^{xiv}	180.000 (1)
O7 ⁱⁱⁱ —Sn1—K2	124.44 (17)	O5 ^{xiii} —K2—O5 ^{xiv}	57.8 (2)
O7 ^{iv} —Sn1—K2	124.43 (17)	O5 ⁱ —K2—O5 ^{xiv}	122.2 (2)
O7 ^v —Sn1—K2	124.43 (17)	O5 ^{viii} —K2—O5 ^{xiv}	57.8 (2)
O8 ^{vi} —Sn2—O8 ^{vii}	92.4 (2)	O5 ⁱⁱ —K2—O5 ^{xiv}	122.2 (2)
O8 ^{vi} —Sn2—O8 ^{viii}	92.4 (2)	O5—K2—O8 ^{xiii}	83.25 (18)
O8 ^{vii} —Sn2—O8 ^{viii}	92.4 (2)	O5 ^{xiii} —K2—O8 ^{xiii}	44.79 (16)
O8 ^{vi} —Sn2—O9 ^{ix}	84.6 (3)	O5 ⁱ —K2—O8 ^{xiii}	135.21 (16)
O8 ^{vii} —Sn2—O9 ^{ix}	100.0 (3)	O5 ^{viii} —K2—O8 ^{xiii}	95.98 (17)
O8 ^{viii} —Sn2—O9 ^{ix}	167.3 (3)	O5 ⁱⁱ —K2—O8 ^{xiii}	84.02 (17)
O8 ^{vi} —Sn2—O9	100.0 (3)	O5 ^{xiv} —K2—O8 ^{xiii}	96.75 (18)
O8 ^{vii} —Sn2—O9	167.3 (3)	O5—K2—O8 ⁱ	96.75 (18)
O8 ^{viii} —Sn2—O9	84.6 (3)	O5 ^{xiii} —K2—O8 ⁱ	135.21 (16)
O9 ^{ix} —Sn2—O9	83.8 (2)	O5 ⁱ —K2—O8 ⁱ	44.79 (16)
O8 ^{vi} —Sn2—O9 ^x	167.3 (3)	O5 ^{viii} —K2—O8 ⁱ	84.02 (17)
O8 ^{vii} —Sn2—O9 ^x	84.6 (3)	O5 ⁱⁱ —K2—O8 ⁱ	95.98 (17)
O8 ^{viii} —Sn2—O9 ^x	100.0 (3)	O5 ^{xiv} —K2—O8 ⁱ	83.25 (18)
O9 ^{ix} —Sn2—O9 ^x	83.8 (2)	O8 ^{xiii} —K2—O8 ⁱ	180.0 (3)
O9—Sn2—O9 ^x	83.8 (2)	O5—K2—O8 ^{viii}	84.02 (17)
O8 ^{vi} —Sn2—K1	123.56 (18)	O5 ^{xiii} —K2—O8 ^{viii}	96.75 (18)
O8 ^{vii} —Sn2—K1	123.56 (18)	O5 ⁱ —K2—O8 ^{viii}	83.25 (18)
O8 ^{viii} —Sn2—K1	123.56 (18)	O5 ^{viii} —K2—O8 ^{viii}	44.79 (16)
O9 ^{ix} —Sn2—K1	50.48 (17)	O5 ⁱⁱ —K2—O8 ^{viii}	135.21 (16)
O9—Sn2—K1	50.48 (17)	O5 ^{xiv} —K2—O8 ^{viii}	95.98 (17)
O9 ^x —Sn2—K1	50.48 (17)	O8 ^{xiii} —K2—O8 ^{viii}	116.25 (7)
O9 ^{xi} —K1—O9 ^{xii}	60.9 (2)	O8 ⁱ —K2—O8 ^{viii}	63.75 (7)
O9 ^{xi} —K1—O9 ^{iv}	60.9 (2)	O5—K2—O8 ⁱⁱ	95.98 (17)
O9 ^{xii} —K1—O9 ^{iv}	60.9 (2)	O5 ^{xiii} —K2—O8 ⁱⁱ	83.25 (18)
O9 ^{xi} —K1—O9 ^{ix}	119.1 (2)	O5 ⁱ —K2—O8 ⁱⁱ	96.75 (18)
O9 ^{xii} —K1—O9 ^{ix}	119.1 (2)	O5 ^{viii} —K2—O8 ⁱⁱ	135.21 (16)
O9 ^{iv} —K1—O9 ^{ix}	179.999 (1)	O5 ⁱⁱ —K2—O8 ⁱⁱ	44.79 (16)
O9 ^{xi} —K1—O9	119.1 (2)	O5 ^{xiv} —K2—O8 ⁱⁱ	84.02 (17)
O9 ^{xii} —K1—O9	179.999 (1)	O8 ^{xiii} —K2—O8 ⁱⁱ	63.75 (7)
O9 ^{iv} —K1—O9	119.1 (2)	O8 ⁱ —K2—O8 ⁱⁱ	116.25 (7)
O9 ^{ix} —K1—O9	60.9 (2)	O8 ^{viii} —K2—O8 ⁱⁱ	180.0 (3)
O9 ^{xi} —K1—O9 ^x	179.999 (1)	O5—K2—O8 ^{xiv}	135.21 (16)
O9 ^{xii} —K1—O9 ^x	119.1 (2)	O5 ^{xiii} —K2—O8 ^{xiv}	95.98 (17)

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09 ^{iv} —K1—09 ^x	119.1 (2)	05 ⁱ —K2—O8 ^{xiv}	84.02 (17)
09 ^{ix} —K1—09 ^x	60.9 (2)	05 ^{viii} —K2—O8 ^{xiv}	96.75 (18)
09—K1—09 ^x	60.9 (2)	05 ⁱⁱ —K2—O8 ^{xiv}	83.25 (18)
09 ^{xi} —K1—O7 ^{ix}	103.41 (17)	05 ^{xiv} —K2—O8 ^{xiv}	44.79 (16)
09 ^{xii} —K1—O7 ^{ix}	72.93 (16)	08 ^{xiii} —K2—O8 ^{xiv}	116.25 (7)
09 ^{iv} —K1—O7 ^{ix}	133.24 (16)	08 ⁱ —K2—O8 ^{xiv}	63.75 (7)
09 ^{ix} —K1—O7 ^{ix}	46.76 (16)	08 ^{viii} —K2—O8 ^{xiv}	116.25 (7)
09—K1—O7 ^{ix}	107.07 (16)	08 ⁱⁱ —K2—O8 ^{xiv}	63.75 (7)
09 ^x —K1—O7 ^{ix}	76.59 (17)	05—K2—O8	44.79 (16)
09 ^{xi} —K1—O7	72.93 (16)	05 ^{xiii} —K2—O8	84.02 (17)
09 ^{xii} —K1—O7	133.23 (16)	05 ⁱ —K2—O8	95.98 (17)
09 ^{iv} —K1—O7	103.41 (17)	05 ^{viii} —K2—O8	83.25 (18)
09 ^{ix} —K1—O7	76.59 (17)	05 ⁱⁱ —K2—O8	96.75 (18)
09—K1—O7	46.76 (16)	05 ^{xiv} —K2—O8	135.21 (16)
09 ^x —K1—O7	107.07 (16)	08 ^{xiii} —K2—O8	63.75 (7)
07 ^{ix} —K1—O7	113.68 (8)	08 ⁱ —K2—O8	116.25 (7)
09 ^{xi} —K1—O7 ^{iv}	76.59 (17)	08 ^{viii} —K2—O8	63.75 (7)
09 ^{xii} —K1—O7 ^{iv}	107.07 (16)	08 ⁱⁱ —K2—O8	116.25 (7)
09 ^{iv} —K1—O7 ^{iv}	46.76 (16)	08 ^{xiv} —K2—O8	180.0
09 ^{ix} —K1—O7 ^{iv}	133.24 (16)	09—P3—O7	106.8 (4)
09—K1—O7 ^{iv}	72.93 (16)	09—P3—O8	108.8 (4)
09 ^x —K1—O7 ^{iv}	103.41 (17)	07—P3—O8	113.5 (4)
07 ^{ix} —K1—O7 ^{iv}	180.0	09—P3—O5	109.6 (4)
07—K1—O7 ^{iv}	66.32 (8)	07—P3—O5	111.2 (3)
09 ^{xi} —K1—O7 ^{xii}	107.07 (16)	08—P3—O5	106.9 (4)
09 ^{xii} —K1—O7 ^{xii}	46.76 (16)	09—P3—K1	44.3 (2)
09 ^{iv} —K1—O7 ^{xii}	76.59 (17)	07—P3—K1	67.0 (3)
09 ^{ix} —K1—O7 ^{xii}	103.41 (17)	08—P3—K1	142.9 (3)
09—K1—O7 ^{xii}	133.24 (16)	05—P3—K1	106.8 (3)
09 ^x —K1—O7 ^{xii}	72.93 (16)	09—P3—K2	88.0 (2)
07 ^{ix} —K1—O7 ^{xii}	66.32 (8)	07—P3—K2	160.5 (3)
07—K1—O7 ^{xii}	180.0	08—P3—K2	71.8 (3)
07 ^{iv} —K1—O7 ^{xii}	113.68 (8)	05—P3—K2	50.5 (2)
09 ^{xi} —K1—O7 ^{xi}	46.76 (16)	K1—P3—K2	121.08 (7)
09 ^{xii} —K1—O7 ^{xi}	76.59 (17)	P3—O5—Sn1	146.4 (4)
09 ^{iv} —K1—O7 ^{xi}	107.07 (16)	P3—O5—K2	105.3 (3)
09 ^{ix} —K1—O7 ^{xi}	72.93 (16)	Sn1—O5—K2	94.2 (2)
09—K1—O7 ^{xi}	103.41 (17)	P3—O7—Sn1 ^v	136.9 (4)
09 ^x —K1—O7 ^{xi}	133.24 (16)	P3—O7—K1	87.9 (3)
07 ^{ix} —K1—O7 ^{xi}	66.33 (8)	Sn1 ^v —O7—K1	128.9 (2)
07—K1—O7 ^{xi}	66.33 (8)	P3—O8—Sn2 ^{vi}	151.1 (4)

$O7^{iv}-K1-O7^{xi}$	113.67 (8)	$P3-O8-K2$	83.2 (3)
$O7^{xii}-K1-O7^{xi}$	113.67 (8)	$Sn2^{vi}-O8-K2$	124.2 (3)
$O9^{xi}-K1-O7^x$	133.24 (16)	$P3-O9-Sn2$	140.7 (4)
$O9^{xii}-K1-O7^x$	103.41 (17)	$P3-O9-K1$	112.7 (3)
$O9^{iv}-K1-O7^x$	72.93 (16)	$Sn2-O9-K1$	93.7 (2)
$O9^{ix}-K1-O7^x$	107.07 (16)		

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

Fig. 1

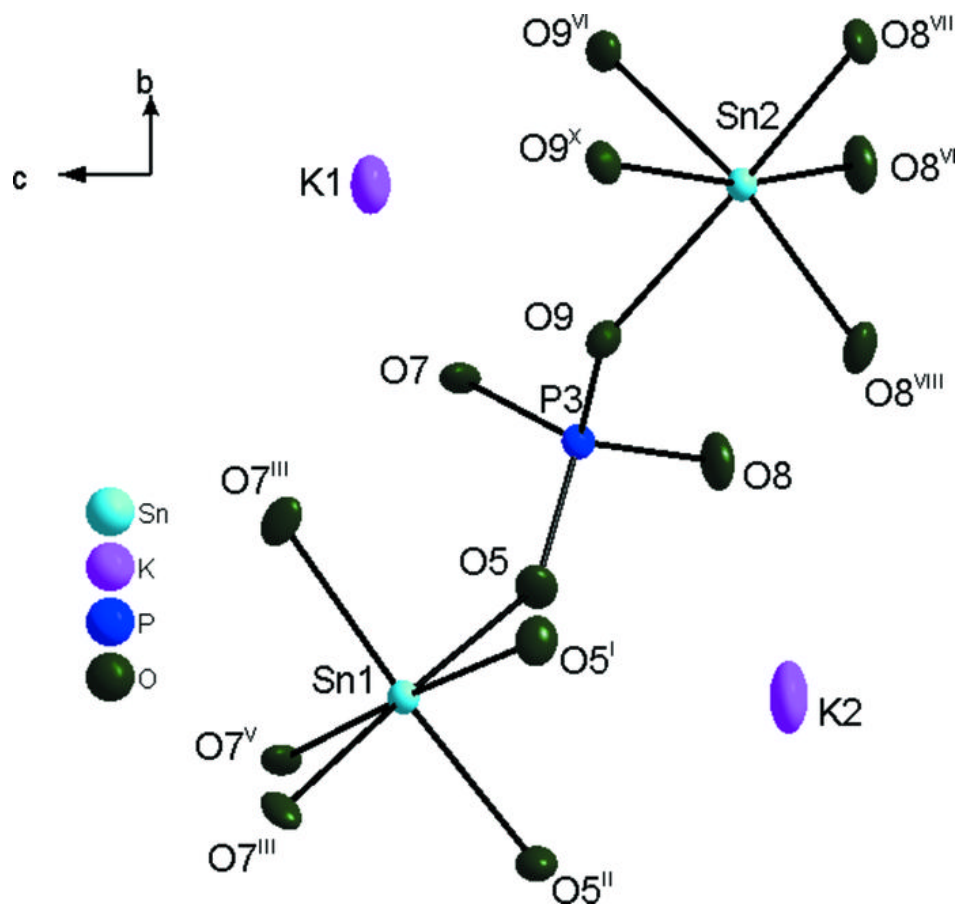


Fig. 2

