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A new langbeinite-type phosphate: $K_2AlSn(PO_4)_3$

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Key indicators: single-crystal X-ray study; T = 296 K; mean σ(P–O) = 0.005 Å; disorder in main residue; R factor = 0.029; wR factor = 0.074; data-to-parameter ratio = 13.7.

Single crystals of the title compound, dipotassium aluminium tin(IV) tris[phosphate(V)], $K_2AlSn(PO_4)_3$, were synthesized by a high temperature reaction in a platinum crucible. In the structure, the Al^{III} and Sn^{IV} atoms occupy the same site on a threefold rotation axis with occupational disorder in a 1:1 ratio. In the three-dimensional structure, Al/SnO_6 octahedra and PO_4 tetrahedra are interconnected *via* their vertices, yielding a $[Al/SnP_3O_{12}]_n$ framework. The K atoms (site symmetry 3) reside in the large cavities delimited by the $[Al/SnP_3O_{12}]_n$ framework, and are surrounded by 12 O atoms.

Related literature

For the mineral langbeinite, $K_2Mg_2(SO_4)_3$, see: Zemann & Zemann (1957). For related langbeinite-type compounds, see: Aatiq *et al.* (2006); Norberg (2002); Ogorodnyk *et al.* (2006); Orlova *et al.* (2003); Zatovsky *et al.* (2007); Zhao *et al.* (2009).

Experimental

Crystal data

$K_2AlSn(PO_4)_3$
M_r = 508.78
Cubic, $P2_13$
a = 9.7980 (8) Å
V = 940.62 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.28 mm^{-1}
T = 296 K
0.15 × 0.05 × 0.05 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.566, T_{max} = 0.815
6146 measured reflections
811 independent reflections
782 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.074
S = 1.18
811 reflections
59 parameters
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}
Absolute structure: Flack (1983), 340 Friedel pairs
Flack parameter: −0.05 (7)

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2112).

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S1. Comment

Langbeinite-type ($K_2Mg_2(SO_4)_3$, Zemann & Zemann, 1957) compounds with the simplest generic formula $A_2B_2(XO_4)_3$ are an important and well studied family of inorganic solids with respect to minerals. Among Langbeinite-based phosphates, whose coordination networks are based on $[M_2(PO_4)_3]$ fragments, may result in diverse structure types due to the 'M_2' sites occupied by various types of tetravalent and bi- or trivalent metal pairs. For example, the structures $K_2M\text{Ti}(PO_4)_3$(M = Y, Yb, Er) (Norberg, 2002), $K_2FeZr(PO_4)_3$ (Orlova *et al.*, 2003), $K_2M\text{Sn}(PO_4)_3$ (M = Fe, Yb) (Aatiq *et al.*, 2006), $K_2AlTi(PO_4)_3$ (Zhao *et al.*, 2009), $K_2FeSn(PO_4)_3$ (Zatovsky *et al.*, 2007) and $K_2Mn_{0.5}Ti_{1.5}(PO_4)_3$ (Ogorodnyk *et al.*, 2006), have been reported. Herein we report the single-crystal growth and structure investigation of title compound $K_2AlSn(PO_4)_3$.

In the structure of title compound, K, Al and Sn atoms lie on the 3-fold rotation axes in 4a positions, while P and O atoms are located at general 12*b* positions. Due to the similar ionic radii of Al and Sn atoms, they occupy the same sites in a substituent disordered manner, denoted as *M* atoms. The three-dimensional structure contains MO_6 octahedra and PO_4 tetrahedra which are connected *via* vertices. Two nearest $[MO_6]$ octahedra are joined to each other by three bridging orthophosphate tetrahedra forming $[Al/SnP_3O_{12}]_n$ framework, which penetrate with large closed cavities. Two independent potassium atoms are located in each cavity. K1 and K2 atoms are 12-coordinated by O atoms.

S2. Experimental

Single crystals of $K_2AlSn(PO_4)_3$ have been prepared by a high-temperature method in air. A powder mixture of K_2CO_3, Al_2O_3, SnO_2 and $NH_4H_2PO_4$ in the molar ratio of K: Al: Sn: P = 10: 1:: 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.

S3. Refinement

The atomic position and anisotropic displacement parameters of Al and Sn in the same sites were constrained to be identical, and the Al/Sn disorder with a relative occupancy of 1/1. The highest peak in the difference electron density map equals to 0.53 e/Å^3 at the distance of 1.09 Å from Al2/Sn2 site while the deepest hole equals to -0.60 e/Å^3 at the distance of 1.78 Å from K2 site.

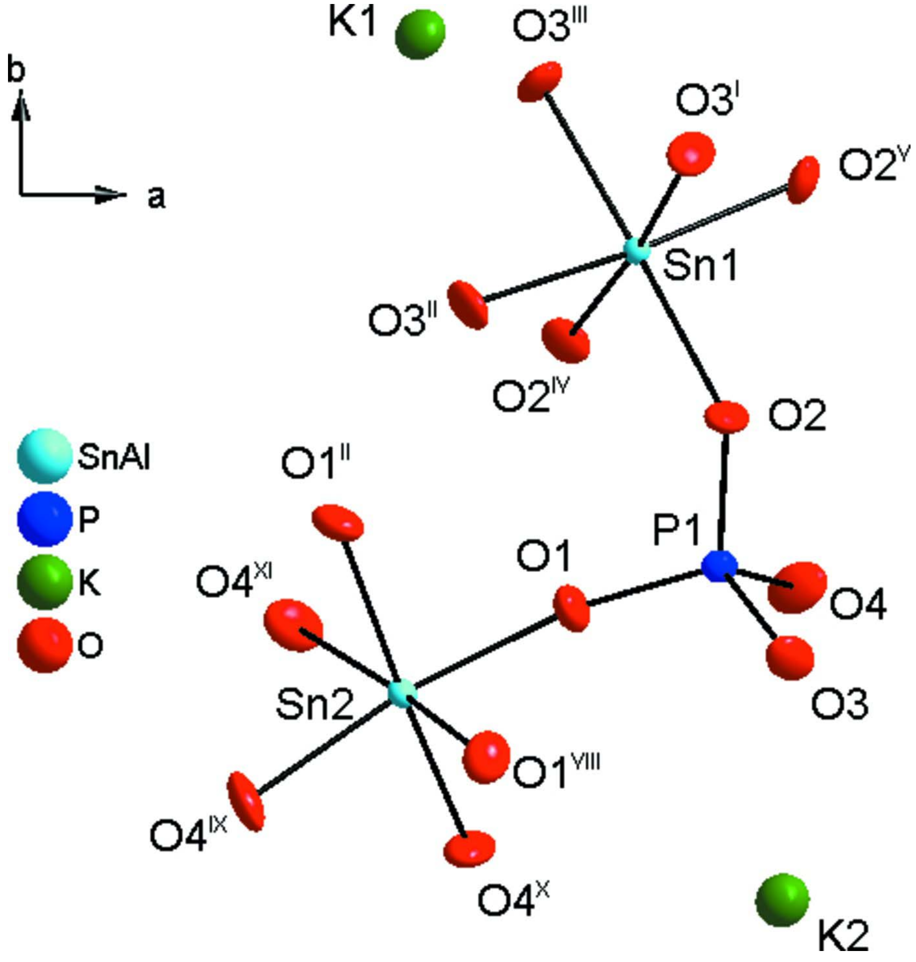

Figure 1

A view of the asymmetric unit of $K_2AlSn(PO_4)_3$ showing the coordination environments of the P and Al/Sn atoms.. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $-x + 1, y + 1/2, -z + 1/2$; (ii) z, x, y; (iii) $-y + 1/2, -z + 1, x - 1/2$; (iv) $-z + 1/2, -x + 1, y - 1/2$; (v) $-y + 1, z + 1/2, -x + 1/2$; (viii) y, z, x; (ix) $-z, x - 1/2, -y + 1/2$; (x) $-y + 1/2, -z, x - 1/2$; (xi) $x - 1/2, -y + 1/2, -z$.]

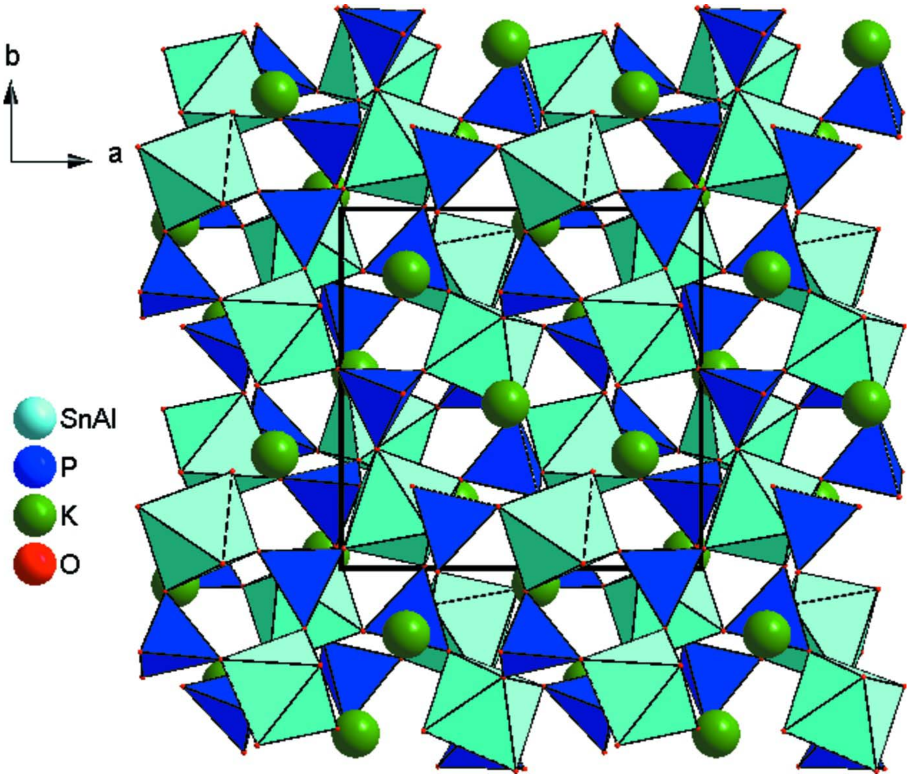

Figure 2

View of the crystal structure of $K_2AlSn(PO_4)_3$ along [010]. PO_4 and Al/SnO_6 units are given in the polyhedral representation.

Dipotassium aluminium tin(IV) tris[phosphate(V)]

Crystal data

$K_2AlSn(PO_4)_3$	$D_x = 3.593$ Mg m^{-3}
$M_r = 508.78$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cubic, $P2_13$	Cell parameters from 2030 reflections
Hall symbol: P 2ac 2ab 3	$\theta = 3.6$–$28.5°$
$a = 9.7980$ (8) Å	$\mu = 4.28$ mm^{-1}
$V = 940.62$ (13) Å^3	$T = 296$ K
$Z = 4$	Prism, colourless
$F(000) = 968$	0.15 × 0.05 × 0.05 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	6146 measured reflections
Radiation source: fine-focus sealed tube	811 independent reflections
Graphite monochromator	782 reflections with $I > 2\sigma(I)$
Detector resolution: 83.33 pixels mm^{-1}	$R_{int} = 0.065$
ω scans	$\theta_{max} = 28.5°$, $\theta_{min} = 2.9°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -13 \rightarrow 6$
	$k = -12 \rightarrow 12$
$T_{min} = 0.566$, $T_{max} = 0.815$	$l = -12 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.074$
$S = 1.18$
811 reflections
59 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0208P)^2 + 3.2535P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.60$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0076 (10)
Absolute structure: Flack (1983), 340 Friedel pairs
Absolute structure parameter: −0.05 (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 (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	0.39682 (6)	0.60318 (6)	0.10318 (6)	0.0091 (2)	0.50
Sn2	0.16412 (6)	0.16412 (6)	0.16412 (6)	0.0104 (2)	0.50
Al1	0.39682 (6)	0.60318 (6)	0.10318 (6)	0.0091 (2)	0.50
Al2	0.16412 (6)	0.16412 (6)	0.16412 (6)	0.0104 (2)	0.50
P1	0.47928 (15)	0.29006 (15)	0.12495 (15)	0.0133 (3)	
K1	0.18221 (14)	0.81779 (14)	0.31779 (14)	0.0268 (5)	
K2	0.54175 (17)	−0.04175 (17)	0.04175 (17)	0.0305 (6)	
O1	0.3329 (4)	0.2484 (4)	0.1004 (5)	0.0231 (9)	
O2	0.4861 (4)	0.4378 (4)	0.1734 (5)	0.0198 (9)	
O3	0.5491 (5)	0.1991 (4)	0.2297 (4)	0.0214 (9)	
O4	0.5569 (5)	0.2684 (5)	−0.0094 (5)	0.0276 (11)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0091 (2)	0.0091 (2)	0.0091 (2)	0.0000 (2)	0.0000 (2)	0.0000 (2)
Sn2	0.0104 (2)	0.0104 (2)	0.0104 (2)	−0.0010 (2)	−0.0010 (2)	−0.0010 (2)
Al1	0.0091 (2)	0.0091 (2)	0.0091 (2)	0.0000 (2)	0.0000 (2)	0.0000 (2)
Al2	0.0104 (2)	0.0104 (2)	0.0104 (2)	−0.0010 (2)	−0.0010 (2)	−0.0010 (2)
P1	0.0142 (7)	0.0131 (7)	0.0126 (7)	0.0002 (5)	−0.0001 (5)	0.0010 (5)
K1	0.0268 (5)	0.0268 (5)	0.0268 (5)	0.0031 (6)	0.0031 (6)	−0.0031 (6)
K2	0.0305 (6)	0.0305 (6)	0.0305 (6)	0.0013 (6)	−0.0013 (6)	0.0013 (6)
O1	0.016 (2)	0.024 (2)	0.030 (2)	−0.0048 (18)	−0.006 (2)	0.0024 (19)

O2	0.021 (2)	0.014 (2)	0.025 (2)	−0.0009 (16)	−0.0065 (19)	−0.0067 (17)
O3	0.025 (2)	0.021 (2)	0.018 (2)	−0.0001 (18)	−0.0077 (18)	0.0088 (18)
O4	0.038 (3)	0.028 (3)	0.017 (2)	0.007 (2)	0.011 (2)	0.003 (2)

Geometric parameters (Å, º)

Sn1—O3^{i}	1.961 (4)	K1—O4^{xii}	3.011 (6)
Sn1—O3^{ii}	1.961 (4)	K1—O4^{xi}	3.011 (6)
Sn1—O3^{iii}	1.961 (4)	K1—O4^{ii}	3.208 (5)
Sn1—O2^{iv}	1.966 (4)	K1—O4^{i}	3.208 (5)
Sn1—O2^{v}	1.966 (4)	K1—O4^{iii}	3.208 (5)
Sn1—O2	1.966 (4)	K2—O2^{xiii}	2.811 (5)
Sn2—O1	1.951 (4)	K2—O2^{xiv}	2.811 (5)
Sn2—O1^{ii}	1.951 (4)	K2—O2^{xv}	2.811 (5)
Sn2—O1^{vi}	1.951 (4)	K2—O3^{ix}	2.994 (5)
Sn2—O4^{vii}	1.960 (5)	K2—O3^{xvi}	2.994 (5)
Sn2—O4^{viii}	1.960 (5)	K2—O3	2.994 (5)
Sn2—O4^{ix}	1.960 (5)	K2—O4^{xvi}	3.084 (5)
P1—O1	1.511 (4)	K2—O4^{ix}	3.084 (5)
P1—O2	1.525 (4)	K2—O4	3.084 (5)
P1—O3	1.521 (4)	O1—K1^{xvii}	2.847 (5)
P1—O4	1.535 (5)	O2—K2^{xviii}	2.811 (5)
K1—O1^{x}	2.847 (5)	O3—Al1^{vi}	1.961 (4)
K1—O1^{xi}	2.847 (5)	O3—Sn1^{vi}	1.961 (4)
K1—O1^{xii}	2.847 (5)	O3—K1^{vi}	2.915 (5)
K1—O3^{ii}	2.916 (5)	O4—Al2^{xvi}	1.960 (5)
K1—O3^{iii}	2.916 (5)	O4—Sn2^{xvi}	1.960 (5)
K1—O3^{i}	2.916 (5)	O4—K1^{xvii}	3.011 (6)
K1—O4^{x}	3.011 (6)	O4—K1^{vi}	3.208 (5)
O3^{i}—Sn1—O3^{ii}	87.42 (19)	O4^{x}—K1—O4^{xii}	86.48 (14)
O3^{i}—Sn1—O3^{iii}	87.42 (19)	O1^{x}—K1—O4^{xi}	52.14 (13)
O3^{ii}—Sn1—O3^{iii}	87.42 (19)	O1^{xi}—K1—O4^{xi}	49.38 (13)
O3^{i}—Sn1—O2^{iv}	175.0 (2)	O1^{xii}—K1—O4^{xi}	114.88 (15)
O3^{ii}—Sn1—O2^{iv}	89.00 (17)	O3^{ii}—K1—O4^{xi}	132.86 (13)
O3^{iii}—Sn1—O2^{iv}	88.90 (18)	O3^{iii}—K1—O4^{xi}	95.45 (12)
O3^{i}—Sn1—O2^{v}	88.90 (19)	O3^{i}—K1—O4^{xi}	140.66 (13)
O3^{ii}—Sn1—O2^{v}	175.0 (2)	O4^{x}—K1—O4^{xi}	86.48 (14)
O3^{iii}—Sn1—O2^{v}	89.00 (17)	O4^{xii}—K1—O4^{xi}	86.48 (14)
O2^{iv}—Sn1—O2^{v}	94.46 (18)	O1^{x}—K1—O4^{ii}	156.33 (13)
O3^{i}—Sn1—O2	88.99 (17)	O1^{xi}—K1—O4^{ii}	55.82 (12)
O3^{ii}—Sn1—O2	88.90 (18)	O1^{xii}—K1—O4^{ii}	86.26 (12)
O3^{iii}—Sn1—O2	175.0 (2)	O3^{ii}—K1—O4^{ii}	46.65 (11)
O2^{iv}—Sn1—O2	94.46 (18)	O3^{iii}—K1—O4^{ii}	88.29 (13)
O2^{v}—Sn1—O2	94.45 (18)	O3^{i}—K1—O4^{ii}	100.74 (13)
O3^{i}—Sn1—K1	52.93 (13)	O4^{x}—K1—O4^{ii}	136.85 (10)
O3^{ii}—Sn1—K1	52.93 (13)	O4^{xii}—K1—O4^{ii}	53.57 (17)
O3^{iii}—Sn1—K1	52.93 (13)	O4^{xi}—K1—O4^{ii}	104.39 (2)

O2^{iv}—Sn1—K1	122.05 (13)
O2^{v}—Sn1—K1	122.05 (13)
O2—Sn1—K1	122.05 (13)
O3^{i}—Sn1—K2^{ii}	129.38 (14)
O3^{ii}—Sn1—K2^{ii}	51.14 (14)
O3^{iii}—Sn1—K2^{ii}	66.00 (13)
O2^{iv}—Sn1—K2^{ii}	45.73 (13)
O2^{v}—Sn1—K2^{ii}	130.02 (13)
O2—Sn1—K2^{ii}	114.01 (13)
K1—Sn1—K2^{ii}	77.229 (18)
O3^{i}—Sn1—K2^{xix}	66.00 (13)
O3^{ii}—Sn1—K2^{xix}	129.38 (14)
O3^{iii}—Sn1—K2^{xix}	51.14 (14)
O2^{iv}—Sn1—K2^{xix}	114.01 (13)
O2^{v}—Sn1—K2^{xix}	45.73 (13)
O2—Sn1—K2^{xix}	130.02 (13)
K1—Sn1—K2^{xix}	77.229 (18)
K2^{ii}—Sn1—K2^{xix}	115.259 (13)
O3^{i}—Sn1—K2^{xviii}	51.14 (14)
O3^{ii}—Sn1—K2^{xviii}	66.00 (13)
O3^{iii}—Sn1—K2^{xviii}	129.38 (14)
O2^{iv}—Sn1—K2^{xviii}	130.02 (13)
O2^{v}—Sn1—K2^{xviii}	114.01 (13)
O2—Sn1—K2^{xviii}	45.73 (13)
K1—Sn1—K2^{xviii}	77.229 (18)
K2^{ii}—Sn1—K2^{xviii}	115.259 (13)
K2^{xix}—Sn1—K2^{xviii}	115.259 (13)
O1—Sn2—O1^{ii}	92.8 (2)
O1—Sn2—O1^{vi}	92.8 (2)
O1^{ii}—Sn2—O1^{vi}	92.8 (2)
O1—Sn2—O4^{vii}	93.7 (2)
O1^{ii}—Sn2—O4^{vii}	82.5 (2)
O1^{vi}—Sn2—O4^{vii}	172.2 (2)
O1—Sn2—O4^{viii}	172.2 (2)
O1^{ii}—Sn2—O4^{viii}	93.7 (2)
O1^{vi}—Sn2—O4^{viii}	82.5 (2)
O4^{vii}—Sn2—O4^{viii}	91.5 (2)
O1—Sn2—O4^{ix}	82.5 (2)
O1^{ii}—Sn2—O4^{ix}	172.2 (2)
O1^{vi}—Sn2—O4^{ix}	93.7 (2)
O4^{vii}—Sn2—O4^{ix}	91.5 (2)
O4^{viii}—Sn2—O4^{ix}	91.5 (2)
O1—Sn2—K1^{xx}	128.15 (13)
O1^{ii}—Sn2—K1^{xx}	49.01 (14)
O1^{vi}—Sn2—K1^{xx}	118.40 (13)
O4^{vii}—Sn2—K1^{xx}	53.89 (16)
O4^{viii}—Sn2—K1^{xx}	59.65 (16)
O4^{ix}—Sn2—K1^{xx}	130.31 (15)
O1^{x}—K1—O4^{i}	86.26 (12)
O1^{xi}—K1—O4^{i}	156.33 (13)
O1^{xii}—K1—O4^{i}	55.82 (12)
O3^{ii}—K1—O4^{i}	88.29 (13)
O3^{iii}—K1—O4^{i}	100.74 (13)
O3^{i}—K1—O4^{i}	46.65 (11)
O4^{x}—K1—O4^{i}	53.57 (17)
O4^{xii}—K1—O4^{i}	104.39 (3)
O4^{xi}—K1—O4^{i}	136.85 (10)
O4^{ii}—K1—O4^{i}	115.74 (6)
O1^{x}—K1—O4^{iii}	55.82 (12)
O1^{xi}—K1—O4^{iii}	86.26 (12)
O1^{xii}—K1—O4^{iii}	156.33 (13)
O3^{ii}—K1—O4^{iii}	100.74 (13)
O3^{iii}—K1—O4^{iii}	46.65 (11)
O3^{i}—K1—O4^{iii}	88.29 (13)
O4^{x}—K1—O4^{iii}	104.39 (2)
O4^{xii}—K1—O4^{iii}	136.85 (10)
O4^{xi}—K1—O4^{iii}	53.57 (17)
O4^{ii}—K1—O4^{iii}	115.74 (6)
O4^{i}—K1—O4^{iii}	115.74 (6)
O2^{xiii}—K2—O2^{xiv}	91.85 (14)
O2^{xiii}—K2—O2^{xv}	91.85 (14)
O2^{xiv}—K2—O2^{xv}	91.85 (14)
O2^{xiii}—K2—O3^{ix}	147.18 (15)
O2^{xiv}—K2—O3^{ix}	56.50 (11)
O2^{xv}—K2—O3^{ix}	81.71 (12)
O2^{xiii}—K2—O3^{xvi}	56.50 (11)
O2^{xiv}—K2—O3^{xvi}	81.71 (12)
O2^{xv}—K2—O3^{xvi}	147.18 (15)
O3^{ix}—K2—O3^{xvi}	119.27 (3)
O2^{xiii}—K2—O3	81.71 (12)
O2^{xiv}—K2—O3	147.18 (15)
O2^{xv}—K2—O3	56.50 (11)
O3^{ix}—K2—O3	119.27 (3)
O3^{xvi}—K2—O3	119.27 (3)
O2^{xiii}—K2—O4^{xvi}	103.66 (12)
O2^{xiv}—K2—O4^{xvi}	82.44 (13)
O2^{xv}—K2—O4^{xvi}	163.58 (13)
O3^{ix}—K2—O4^{xvi}	82.31 (13)
O3^{xvi}—K2—O4^{xvi}	47.30 (12)
O3—K2—O4^{xvi}	130.38 (15)
O2^{xiii}—K2—O4^{ix}	163.58 (13)
O2^{xiv}—K2—O4^{ix}	103.66 (12)
O2^{xv}—K2—O4^{ix}	82.44 (13)
O3^{ix}—K2—O4^{ix}	47.30 (12)
O3^{xvi}—K2—O4^{ix}	130.38 (15)
O3—K2—O4^{ix}	82.31 (13)

O1—Sn2—K1^{xxi}	118.40 (13)
O1^{ii}—Sn2—K1^{xxi}	128.15 (13)
O1^{vi}—Sn2—K1^{xxi}	49.01 (14)
O4^{vii}—Sn2—K1^{xxi}	130.31 (15)
O4^{viii}—Sn2—K1^{xxi}	53.89 (16)
O4^{ix}—Sn2—K1^{xxi}	59.65 (16)
K1^{xx}—Sn2—K1^{xxi}	113.210 (15)
O1—Sn2—K1^{xvii}	49.01 (14)
O1^{ii}—Sn2—K1^{xvii}	118.40 (13)
O1^{vi}—Sn2—K1^{xvii}	128.15 (13)
O4^{vii}—Sn2—K1^{xvii}	59.65 (16)
O4^{viii}—Sn2—K1^{xvii}	130.31 (15)
O4^{ix}—Sn2—K1^{xvii}	53.89 (16)
K1^{xx}—Sn2—K1^{xvii}	113.210 (15)
K1^{xxi}—Sn2—K1^{xvii}	113.210 (15)
O1—P1—O2	110.3 (3)
O1—P1—O3	112.1 (3)
O2—P1—O3	109.1 (3)
O1—P1—O4	107.2 (3)
O2—P1—O4	112.1 (3)
O3—P1—O4	105.9 (3)
O1—P1—K1^{vi}	168.93 (19)
O2—P1—K1^{vi}	80.16 (17)
O3—P1—K1^{vi}	59.55 (18)
O4—P1—K1^{vi}	70.5 (2)
O1—P1—K2	82.78 (18)
O2—P1—K2	166.53 (19)
O3—P1—K2	61.42 (18)
O4—P1—K2	64.79 (19)
K1^{vi}—P1—K2	86.56 (5)
O1—P1—K1^{xvii}	50.43 (19)
O2—P1—K1^{xvii}	124.36 (19)
O3—P1—K1^{xvii}	126.57 (19)
O4—P1—K1^{xvii}	56.9 (2)
K1^{vi}—P1—K1^{xvii}	126.95 (5)
K2—P1—K1^{xvii}	66.07 (6)
O1—P1—K2^{xviii}	102.1 (2)
O2—P1—K2^{xviii}	45.40 (18)
O3—P1—K2^{xviii}	71.80 (18)
O4—P1—K2^{xviii}	148.7 (2)
K1^{vi}—P1—K2^{xviii}	82.58 (4)
K2—P1—K2^{xviii}	130.74 (6)
K1^{xvii}—P1—K2^{xviii}	149.53 (5)
O1^{x}—K1—O1^{xi}	100.53 (12)
O1^{x}—K1—O1^{xii}	100.53 (12)
O1^{xi}—K1—O1^{xii}	100.53 (12)
O1^{x}—K1—O3^{ii}	149.59 (14)
O1^{xi}—K1—O3^{ii}	96.38 (13)
O4^{xvi}—K2—O4^{ix}	83.98 (16)
O2^{xiii}—K2—O4	82.44 (13)
O2^{xiv}—K2—O4	163.58 (13)
O2^{xv}—K2—O4	103.66 (12)
O3^{ix}—K2—O4	130.38 (15)
O3^{xvi}—K2—O4	82.31 (13)
O3—K2—O4	47.30 (12)
O4^{xvi}—K2—O4	83.98 (16)
O4^{ix}—K2—O4	83.98 (16)
O2^{xiii}—K2—P1	93.94 (9)
O2^{xiv}—K2—P1	169.50 (10)
O2^{xv}—K2—P1	79.23 (9)
O3^{ix}—K2—P1	116.07 (10)
O3^{xvi}—K2—P1	108.78 (10)
O3—K2—P1	26.50 (8)
O4^{xvi}—K2—P1	104.63 (13)
O4^{ix}—K2—P1	69.91 (10)
O4—K2—P1	26.76 (9)
O2^{xiii}—K2—P1^{ix}	169.50 (10)
O2^{xiv}—K2—P1^{ix}	79.23 (9)
O2^{xv}—K2—P1^{ix}	93.94 (9)
O3^{ix}—K2—P1^{ix}	26.50 (8)
O3^{xvi}—K2—P1^{ix}	116.07 (10)
O3—K2—P1^{ix}	108.78 (10)
O4^{xvi}—K2—P1^{ix}	69.91 (10)
O4^{ix}—K2—P1^{ix}	26.76 (9)
O4—K2—P1^{ix}	104.63 (13)
P1—K2—P1^{ix}	95.73 (6)
O2^{xiii}—K2—P1^{xvi}	79.23 (9)
O2^{xiv}—K2—P1^{xvi}	93.94 (9)
O2^{xv}—K2—P1^{xvi}	169.50 (10)
O3^{ix}—K2—P1^{xvi}	108.78 (10)
O3^{xvi}—K2—P1^{xvi}	26.50 (8)
O3—K2—P1^{xvi}	116.07 (10)
O4^{xvi}—K2—P1^{xvi}	26.76 (9)
O4^{ix}—K2—P1^{xvi}	104.63 (13)
O4—K2—P1^{xvi}	69.91 (10)
P1—K2—P1^{xvi}	95.73 (6)
P1^{ix}—K2—P1^{xvi}	95.73 (6)
P1—O1—Sn2	150.2 (3)
P1—O1—K1^{xvii}	105.4 (2)
Sn2—O1—K1^{xvii}	99.85 (17)
P1—O2—Sn1	130.9 (3)
P1—O2—K2^{xviii}	111.9 (2)
Sn1—O2—K2^{xviii}	104.22 (16)
P1—O3—Al1^{vi}	164.9 (3)
P1—O3—Sn1^{vi}	164.9 (3)
Al1^{vi}—O3—Sn1^{vi}	0.00 (5)

O1^{xii}—K1—O3^{ii}	100.99 (13)	P1—O3—K1^{vi}	93.7 (2)
O1^{x}—K1—O3^{iii}	96.38 (13)	Al1^{vi}—O3—K1^{vi}	94.60 (17)
O1^{xi}—K1—O3^{iii}	100.99 (13)	Sn1^{vi}—O3—K1^{vi}	94.60 (17)
O1^{xii}—K1—O3^{iii}	149.59 (14)	P1—O3—K2	92.1 (2)
O3^{ii}—K1—O3^{iii}	55.40 (14)	Al1^{vi}—O3—K2	98.18 (17)
O1^{x}—K1—O3^{i}	100.99 (13)	Sn1^{vi}—O3—K2	98.18 (17)
O1^{xi}—K1—O3^{i}	149.59 (14)	K1^{vi}—O3—K2	103.77 (14)
O1^{xii}—K1—O3^{i}	96.38 (13)	P1—O4—Al2^{xvi}	152.0 (3)
O3^{ii}—K1—O3^{i}	55.40 (14)	P1—O4—Sn2^{xvi}	152.0 (3)
O3^{iii}—K1—O3^{i}	55.40 (14)	Al2^{xvi}—O4—Sn2^{xvi}	0.000 (18)
O1^{x}—K1—O4^{x}	49.38 (13)	P1—O4—K1^{xvii}	97.8 (2)
O1^{xi}—K1—O4^{x}	114.88 (15)	Al2^{xvi}—O4—K1^{xvii}	94.39 (18)
O1^{xii}—K1—O4^{x}	52.14 (13)	Sn2^{xvi}—O4—K1^{xvii}	94.39 (18)
O3^{ii}—K1—O4^{x}	140.66 (13)	P1—O4—K2	88.5 (2)
O3^{iii}—K1—O4^{x}	132.86 (13)	Al2^{xvi}—O4—K2	118.9 (2)
O3^{i}—K1—O4^{x}	95.45 (12)	Sn2^{xvi}—O4—K2	118.9 (2)
O1^{x}—K1—O4^{xii}	114.88 (15)	K1^{xvii}—O4—K2	77.14 (14)
O1^{xi}—K1—O4^{xii}	52.14 (13)	P1—O4—K1^{vi}	82.7 (2)
O1^{xii}—K1—O4^{xii}	49.38 (13)	Al2^{xvi}—O4—K1^{vi}	88.54 (19)
O3^{ii}—K1—O4^{xii}	95.45 (12)	Sn2^{xvi}—O4—K1^{vi}	88.54 (19)
O3^{iii}—K1—O4^{xii}	140.66 (13)	K1^{xvii}—O4—K1^{vi}	172.37 (18)
O3^{i}—K1—O4^{xii}	132.86 (12)	K2—O4—K1^{vi}	95.27 (14)

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2; (ii) *z*, *x*, *y*; (iii) −*y*+1/2, −*z*+1, *x*−1/2; (iv) −*z*+1/2, −*x*+1, *y*−1/2; (v) −*y*+1, *z*+1/2, −*x*+1/2; (vi) *y*, *z*, *x*; (vii) *x*−1/2, −*y*+1/2, −*z*; (viii) −*z*, *x*−1/2, −*y*+1/2; (ix) −*y*+1/2, −*z*, *x*−1/2; (x) *y*, *z*+1, *x*; (xi) −*z*, *x*+1/2, −*y*+1/2; (xii) −*x*+1/2, −*y*+1, *z*+1/2; (xiii) −*z*+1, *x*−1/2, −*y*+1/2; (xiv) −*y*+1, *z*−1/2, −*x*+1/2; (xv) −*x*+1, *y*−1/2, −*z*+1/2; (xvi) *z*+1/2, −*x*+1/2, −*y*; (xvii) *z*, *x*, *y*−1; (xviii) −*z*+1/2, −*x*+1, *y*+1/2; (xix) *x*, *y*+1, *z*; (xx) *y*−1, *z*, *x*; (xxi) *x*, *y*−1, *z*.