

Table 35A-11-001. KSnOPO₄. Atomic coordinates and temperature parameters [\AA^2] [90Tho]. For definition of U_{ij} , see Eq. (d) in Introduction. OS(1): oxygen of Sn(1) side. OS(2): oxygen of Sn(2) side.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
K(1)	0.3753(1)	0.7771(2)	0.6983(0)	0.0171(9)	0.0089(7)	0.0243(8)	-0.0003(6)	-0.0038(5)	0.0050(7)
K(2)	0.1089(1)	0.6930(3)	0.9393(2)	0.0126(8)	0.0210(7)	0.0307(8)	0.0001(8)	0.0001(6)	0.0063(7)
Sn(1)	0.2487(0)	0.2544(1)	0.7496(2)	0.0025(2)	0.0033(2)	0.0038(2)	-0.0003(1)	-0.0006(1)	-0.0004(1)
Sn(2)	0.3729(0)	0.4976(1)	0.0002(2)	0.0028(2)	0.0019(2)	0.0036(2)	-0.0006(1)	-0.0003(3)	0.0003(2)
P(1)	0.5012(1)	0.3411(2)	0.7520(3)	0.0033(8)	0.0049(6)	0.0057(5)	-0.003(1)	0.0012(4)	0.0004(8)
P(2)	0.1758(1)	0.5017(3)	0.4970(4)	0.0038(8)	0.0030(6)	0.0062(5)	0.0005(6)	-0.004(1)	-0.0014(8)
O(1)	0.4878(6)	0.4883(7)	0.8656(6)	0.009(1)	0.009(1)	0.010(1)	-0.0029(9)	0.0037(8)	-0.004(1)
O(2)	0.9856(6)	0.9782(7)	0.1371(6)	0.009(1)	0.009(1)	0.010(1)	0.0029(9)	-0.0037(8)	-0.004(1)
O(3)	0.4083(4)	0.2051(7)	0.7293(4)	0.002(1)	0.010(1)	0.014(1)	-0.003(1)	-0.0022(8)	0.001(1)
O(4)	0.9086(4)	0.7030(7)	0.2734(4)	0.002(1)	0.010(1)	0.014(1)	0.003(1)	0.0022(8)	0.001(1)
O(5)	0.1062(4)	0.3160(6)	0.4761(4)	0.011(1)	0.007(1)	0.008(1)	-0.001(1)	-0.0031(7)	0.000(1)
O(6)	0.6074(4)	0.8137(7)	0.5233(4)	0.011(1)	0.007(1)	0.008(1)	0.001(1)	0.0031(7)	0.000(1)
OS(1)	0.2285(6)	0.9827(8)	0.3644(6)	0.009(1)	0.007(1)	0.011(1)	-0.002(1)	0.0048(8)	0.000(1)
OS(2)	0.7347(6)	0.4659(9)	0.6266(6)	0.009(1)	0.007(1)	0.011(1)	0.002(1)	-0.0048(8)	0.000(1)
O(7)	0.2450(5)	0.5318(9)	0.3843(7)	0.010(1)	0.012(1)	0.012(1)	0.006(1)	0.0033(8)	0.002(1)
O(8)	0.7485(5)	0.0282(9)	0.6085(7)	0.010(1)	0.012(1)	0.012(1)	-0.006(1)	-0.0033(8)	0.002(1)

Table 35A-11-002. KSnOPO₄. Bond lengths [\AA^2] [90Tho]. OS(1): oxygen of Sn(1) side. OS(2): oxygen of Sn(2) side.

Sn(2)O ₆ octahedron		Sn(1)O ₆ octahedron	
Sn(2)–O(1)	2.091(7)	Sn(1)–O(3)	2.134(5)
Sn(2)–O(2)	2.093(7)	Sn(1)–O(4)	2.102(5)
Sn(2)–OS(1)	1.978(6)	Sn(1)–OS(1)	1.957(5)
Sn(2)–OS(2)	1.975(7)	Sn(1)–OS(2)	1.961(5)
Sn(2)–O(5)	2.111(6)	Sn(1)–O(7)	2.051(6)
Sn(2)–O(6)	2.064(5)	Sn(1)–O(8)	2.076(7)
O(1)–O(2)	2.923(6)	O(3)–OS(1)	2.937(7)
O(1)–O(5)	2.740(7)	O(3)–OS(2)	2.767(6)
O(1)–O(6)	2.884(8)	O(3)–O(7)	2.848(7)
O(1)–OS(1)	2.843(8)	O(3)–O(8)	3.021(9)
O(2)–OS(2)	2.899(9)	O(4)–OS(1)	2.834(8)
O(2)–O(5)	2.850(7)	O(4)–OS(2)	2.995(8)
O(2)–O(6)	2.790(7)	O(4)–O(7)	3.006(9)
OS(1)–O(5)	2.958(9)	O(4)–O(8)	2.949(7)
OS(1)–OS(2)	2.838(8)	O(7)–OS(1)	2.959(7)
OS(2)–O(6)	3.031(8)	O(7)–OS(2)	2.779(9)
OS(2)–O(5)	2.974(9)	O(8)–OS(1)	2.764(8)
OS(1)–O(6)	3.032(9)	O(8)–OS(2)	2.869(6)
P(1)O ₄ tetrahedron		P(2)O ₄ tetrahedron	
P(1)–O(1)	1.562(6)	P(2)–O(5)	1.535(5)
P(1)–O(2)	1.535(7)	P(2)–O(6)	1.529(6)
P(1)–O(3)	1.530(5)	P(2)–O(7)	1.527(8)
P(1)–O(4)	1.506(6)	P(2)–O(8)	1.545(7)
O(1)–O(2)	2.480(7)	O(5)–O(6)	2.469(8)
O(1)–O(3)	2.579(8)	O(5)–O(7)	2.508(7)
O(1)–O(4)	2.510(8)	O(5)–O(8)	2.560(8)
O(2)–O(3)	2.471(6)	O(6)–O(7)	2.553(6)
O(2)–O(4)	2.529(7)	O(6)–O(8)	2.497(7)
O(3)–O(4)	2.453(7)	O(7)–O(8)	2.441(6)
K(1)O ₈ cage		K(2)O ₈ cage	
K(1)–O(1)	2.995(7)	K(2)–O(1)	2.736(6)
K(1)–O(2)	2.753(4)	K(2)–O(2)	3.256(8)
K(1)–O(3)	2.845(5)	K(2)–O(4)	3.148(5)
K(1)–OS(1)	2.955(5)	K(2)–OS(1)	2.664(5)
K(1)–OS(2)	2.611(6)	K(2)–OS(2)	3.058(7)
K(1)–O(5)	3.005(4)	K(2)–O(5)	2.856(6)
K(1)–O(7)	3.042(4)	K(2)–O(7)	2.987(6)
K(1)–O(8)	2.770(7)	K(2)–O(8)	3.182(7)
		K(2)–O(3)	3.123(7)

Table 35A-11-003. KSnOPO₄. Bond lengths of SnO₆ octahedra compared with those of KTiOPO₄ and RbTiOPO₄ [89Tho]. OT(1): oxygen of Ti(1) side. OT(2): oxygen of Ti(2) side. OS(1): oxygen of Sn(1) side. OS(2): oxygen of Sn(2) side.

Bond	KTP [Å]	RTP [Å]	Bond	KSP [Å]
Ti(1)–O(1)	2.150	2.148	Sn(1)–O(1)	2.091
Ti(1)–O(2)	1.958	1.949	Sn(2)–O(2)	2.093
Ti(1)–OT(1)	1.981	1.952	Sn(1)–OS(1)	1.978
Ti(1)–OT(2)	1.716	1.717	Sn(1)–OS(2)	1.975
Ti(1)–O(5)	2.043	2.072	Sn(1)–O(5)	2.112
Ti(1)–O(6)	1.987	2.016	Sn(1)–O(6)	2.063
Ti(2)–O(3)	2.044	2.061	Sn(2)–O(3)	2.134
Ti(2)–O(4)	1.981	2.005	Sn(2)–O(4)	2.102
Ti(2)–OT(1)	1.733	1.746	Sn(2)–OS(1)	1.957
Ti(2)–OT(2)	2.092	2.089	Sn(2)–OS(2)	1.961
Ti(2)–O(7)	1.964	1.971	Sn(2)–O(7)	2.052
Ti(2)–O(8)	1.991	1.995	Sn(2)–O(8)	2.076

Table 35A-11-004. KSnOPO₄. Comparison of the structure with that of KTiOPO₄ [90Tho]. Displacements of atoms in KTiOPO₄ and KSnOPO₄ from high-symmetry (Pnan) positions. OS(1): oxygen of Sn(1) side. OT(1): oxygen of Ti(1) side.

	Position in room-temperature structure – ($\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$) for origin shift			Positon in high-temperature structure (space group Pnan)	Displacement $\Delta x, \Delta y, \Delta z$ when n -glide plane is assumed to pass through $(0, 0, \frac{1}{4})$ [Å]		Displacement Δz when $\Sigma_i m_i(z_i - z_c)$ is minimized [Å]	
KTP								
Ti(1)	0.1229,	0.2496,	0.7496	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$ [4(d)] ($x = 0.3771$)	0,	−0.002,	−0.004	−0.046
Ti(2)	0.9966,	0.0195,	0.4984	$0, 0, \frac{1}{2}$ [4(b)]	−0.043,	0.125,	−0.017	−0.059
K(1)	0.1281,	0.5306,	0.4380	Average (x, y, z) for general position	0.106,	0.062,	0.635	+0.599
K(2)	0.6447,	0.0501,	0.1820		0.1364	0.5403	0.378	
(pseudo n glide related to K1 above)								
P(1)	0.2481,	0.0863,	0.4897	$\frac{1}{4}, -y + \frac{1}{2}, \frac{1}{2}$ [4(c)]	−0.024,	0,	−0.109	−0.151
P(2)	0.9308,	0.2520,	0.2372	$x, \frac{1}{4}, \frac{1}{4}$ [4(d)]	0,	0.013,	−0.135	−0.178
O(1)	0.2359,	0.2367,	0.5997	Average (x, y, z) for general position	0.097,	0.067,	0.176	−0.217
O(2)	0.7397,	0.7158,	0.8670	0.2378,				
O(3)	0.1504,	0.9486,	0.4708	0.2262,	0.001,	0.050,	0.107	−0.150
O(4)	0.6506,	0.4430,	0.0089	0.1505,				
OT(1)	0.9748,	0.7153,	0.1061	0.9408,	0.010,	0.021,	0.181	−0.223
OT(2)	0.4732,	0.2087,	0.3597	0.7120,				
O(5)	0.8626,	0.0606,	0.2084	0.1232	0.009,	0.001,	0.157	−0.200
O(6)	0.3613,	0.5582,	0.2617	0.0594,				
O(7)	0.0025,	0.2902,	0.1218	0.2233	0.001,	0.007,	0.145	−0.187
O(8)	0.5028,	0.7881,	0.3508	0.8619,				
				0.0026,				
				0.2891,				
				0.1355				
								(continued)

(continued)

Table 35A-11-004 (continued)

	Position in room-temperature structure – ($\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$) for origin shift		Position in high-temperature structure (space group Pnan)		Displacement $\Delta x, \Delta y, \Delta z$ when n -glide plane is assumed to pass through $(0, 0, \frac{1}{4})$ [Å]		Displacement Δz when $\sum_i m_i(z_i - z_z)$ is minimized [Å]	
KSP								
Sn(1)	0.1229,	0.2476,	0.7502	$\bar{x} + \frac{1}{2}, \frac{1}{4}, \frac{3}{4} [4(d)]$	0,	–0.016,	0.002	–0.115
Sn(2)	0.9987,	0.0044,	0.4996	$0, 0, \frac{1}{2} [4(b)]$	–0.017,	0.029,	–0.004	–0.117
P(1)	0.2512,	0.0911,	0.5020	$\frac{1}{4}, -y + \frac{1}{2}, \frac{1}{2} [4(c)]$	0.016,	0,	0.021	–0.092
P(2)	0.9258,	0.2517,	0.2470	$x, \frac{1}{4}, \frac{1}{4} [4(d)]$	0,	0.011,	–0.032	–0.145
K(1)	0.1253,	0.5271,	0.4483	} 0.1332,	0.542,	0.097,	0.739	+0.625
K(2)	0.6411,	0.0569,	0.1893					
O(1)	0.2378,	0.2383,	0.6156	} 0.2367,	0.2332,	0.033	0.015	–0.098
O(2)	0.7356,	0.7282,	0.8871					
O(3)	0.1583,	0.9551,	0.4793	} 0.1584,	0.9540,	0.007,	0.014	–0.099
O(4)	0.6586,	0.4530,	0.0234					
OS(1)	0.9785,	0.7327,	0.1144	} 0.9816,	0.7243,	0.055,	0.048	–0.065
OS(2)	0.4847,	0.2159,	0.3766					
O(5)	0.8652,	0.0660,	0.2261	} 0.8613,	0.0648,	0.008,	0.003	–0.110
O(6)	0.3574,	0.5637,	0.2733					
O(7)	0.9950,	0.2818,	0.1343	} 0.9967,	0.2800,	0.012,	0.039	–0.074
O(8)	0.4985,	0.7782,	0.3585					