Table 35A-2-001. $KSbOSiO_4$. Atomic coordinates and temperature parameters [94Fav]. T = 400 °C (phase I). B: isotropic temperature parameter defined in Eq. (e) in Introduction. U_{ij}: anisotropic temperature parameter defined in Eq. (d) in Introduction.

(a)	x	y	z	Occupancy	B [Å^2]
Sb(1)	0.13086(6)	0.250	0.750	1	0.681(9)
Sb(2)	0.000	0.000	0.000	1	0.709(9)
Si(1)	0.250	0.0767(6)	0.000	1	0.84(5)
Si(2)	0.9305(3)	0.250	0.250	1	0.90(5)
O(1)	0.2625(5)	0.226(1)	0.1209(7)	1	1.5(1)
O(2)	0.1492(5)	0.931(1)	1.0197(7)	1	1.4(1)
O(3)	0.8595(6)	0.052(1)	0.2801(7)	1	1.5(1)
O(4)	0.0090(6)	0.294(1)	0.3671(7)	1	1.4(1)
O(5)	0.9768(5)	0.721(1)	0.3769(7)	1	1.7(1)
K(1)	0.1348(6)	0.532(1)	0.0814(9)	0.45(2)	4.5(2)
K(2)	0.1407(6)	0.547(1)	0.1663(9)	0.55(2)	4.3(2)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sb(1)	0.0087(2)	0.0089(2)	0.0083(2)	0	0	0.0013(4)
Sb(2)	0.0084(2)	0.0106(2)	0.0080(2)	–0.0007(3)	0.0005(3)	–0.0000(4)
Si(1)	0.008(1)	0.011(1)	0.013(1)	0	–0.003(1)	0
Si(2)	0.013(1)	0.010(1)	0.011(1)	0	0	–0.001(2)
O(1)	0.016(3)	0.025(3)	0.017(3)	0.002(3)	–0.010(2)	–0.011(3)
O(2)	0.007(2)	0.024(3)	0.023(4)	–0.001(3)	–0.001(2)	0.002(3)
O(3)	0.019(3)	0.011(3)	0.026(4)	–0.002(3)	0.006(3)	0.002(3)
O(4)	0.019(3)	0.018(3)	0.016(3)	0.004(3)	–0.002(3)	–0.009(2)
O(5)	0.014(3)	0.028(4)	0.021(3)	–0.006(3)	–0.010(2)	0.004(3)
K(1)	0.040(3)	0.031(3)	0.100(6)	0.012(3)	0.026(4)	0.016(4)
K(2)	0.032(3)	0.045(4)	0.086(6)	0.011(3)	0.004(4)	0.007(4)

Table 35A-2-002. $KSbOSiO_4$. Atomic coordinates and temperature parameters [90Cro]. Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent temperature parameter. B: isotropic temperature parameter defined in Eq. (e) in Introduction.

Atom	Position	x	y	z	B [Å^2]
Sb(1)	4a	0.38119(3)	0.5002(2)	0.0	0.446(5)
Sb(2)	4a	0.24768(7)	0.2526(2)	0.2488(2)	0.460(5)
Si(1)	4a	0.4998(4)	0.3271(3)	0.2488(8)	0.55(2)
Si(2)	4a	0.1815(1)	0.5039(9)	0.4994(7)	0.54(2)
K(1)	4a	0.3816(2)	0.7766(4)	0.3107(2)	1.86(4)
K(2)	4a	0.1073(2)	0.6962(4)	0.0656(3)	1.95(4)
O(1)	4a	0.4846(5)	0.491(1)	0.1344(6)	0.97(9)*
O(2)	4a	0.5082(4)	0.4661(8)	0.3765(5)	0.35(8)*
O(3)	4a	0.3966(4)	0.1834(9)	0.2677(5)	0.49(8)*
O(4)	4a	0.5993(5)	0.194(1)	0.2318(6)	1.0(1)*
O(5)	4a	0.1112(5)	0.303(1)	0.5314(5)	0.9(1)*
O(6)	4a	0.1077(5)	0.6979(9)	0.4723(5)	0.63(9)*
O(7)	4a	0.2558(5)	0.5380(9)	0.6188(5)	0.68(9)*
O(8)	4a	0.2626(5)	0.452(1)	0.3849(6)	0.8(1)*
O(9)	4a	0.2229(4)	0.980(1)	0.6322(5)	0.39(8)*
O(10)	4a	0.2286(4)	0.0390(9)	0.3777(5)	0.45(9)*

Table 35A-2-003. $KSbOSiO_4$. Anisotropic temperature parameters [$\cdot 10^{-3}$ Å^2] [90Cro]. U_{ij}: anisotropic temperature parameter defined in Eq. (d) in Introduction.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sb(1)	5.7(1)	6.9(1)	4.3(1)	0.5(8)	0.7(5)	0.8(2)
Sb(2)	5.7(1)	7.4(1)	4.4(1)	–0.4(2)	0.3(2)	–0.2(2)
Si(1)	6.0(6)	8.6(6)	6.3(6)	–2(2)	–0.1(7)	–2(3)
Si(2)	8.1(6)	6.0(6)	6.2(6)	0(2)	5(2)	–0.1(8)
K(1)	24(1)	15(1)	32(1)	6.4(9)	6.8(9)	4.9(9)
K(2)	13.8(9)	24(1)	36(1)	6.0(9)	0.1(9)	3(1)

Table 35A-2-004. $KSbOSiO_4$. Interatomic distances [Å] and bond angles [°] for the coordination polyhedra [90Cro].

$Sb(1)O_6$ octahedron						
Sb(1)	O(1)	O(2)	O(5)	O(6)	O(9)	O(10)
O(1)	1.961(9)	2.753(7)	2.61(1)	2.83(1)	2.70(1)	3.90(1)
O(2)	89.3(2)	1.958(8)	2.74(1)	2.73(1)	3.91(1)	2.87(1)
O(5)	82.8(4)	88.1(4)	1.99(1)	3.967(6)	2.76(1)	2.81(1)
O(6)	91.5(4)	87.6(4)	172.9(2)	1.99(1)	2.91(1)	2.89(1)
O(9)	87.2(3)	175.5(3)	88.8(4)	95.2(4)	1.955(8)	2.729(7)
O(10)	172.9(4)	94.5(3)	91.2(4)	94.7(4)	88.8(2)	1.946(9)
$Sb(2)O_6$ octahedron						
Sb(2)	O(3)	O(4)	O(7)	O(8)	O(9)	O(10)
O(3)	2.00(1)	3.979(6)	2.71(2)	2.76(2)	2.86(1)	2.65(1)
O(4)	178.9(6)	1.98(1)	2.87(2)	2.82(2)	2.76(1)	2.91(1)
O(7)	86.2(5)	93.50(5)	1.96(1)	3.902(6)	2.90(1)	2.76(1)
O(8)	88.7(5)	91.6(5)	174.4(6)	1.95(1)	2.69(1)	2.71(2)
O(9)	92.5(4)	88.7(4)	95.4(4)	87.1(5)	1.96(1)	3.917(6)
O(10)	83.9(4)	95.0(5)	89.3(4)	87.9(4)	173.9(5)	1.961(9)
$Si(1)O_4$ tetrahedron						
Si(1)	O(1)	O(2)	O(3)	O(4)		
O(1)	1.62(1)	2.593(7)	2.70(1)	2.69(2)		
O(2)	105.6(4)	1.63(1)	2.61(1)	2.66(1)		
O(3)	111.1(6)	105.4(6)	1.65(1)	2.663(7)		
O(4)	113.0(7)	111.1(6)	110.2(2)	1.60(1)		
$Si(2)O_4$ tetrahedron						
Si(2)	O(5)	O(6)	O(7)	O(8)		
O(5)	1.63(1)	2.634(6)	2.59(2)	2.69(2)		
O(6)	109.2(3)	1.61(1)	2.68(2)	2.73(2)		
O(7)	106.4(7)	113.1(7)	1.61(1)	2.545(7)		
O(8)	110.6(7)	114.2(7)	103.0(3)	1.64(1)		
K–O distances < 3.1 Å						
	O(1)	O(2)	O(3)	O(4)	O(5)	
K(1)	2.95(1)	2.691(8)	2.68(1)		2.97(1)	
K(2)	2.68(1)	3.056(8)		3.03(1)	2.87(1)	
	O(6)	O(7)	O(8)	O(9)	O(10)	
K(1)			2.73(1)	3.020(9)	2.71(1)	
K(2)		2.90(1)	3.05(1)	2.707(9)	3.09(1)	