

Table 35A-15-001. KSbOGeO₄. Atomic coordinates and anisotropic temperature parameters [91Bel]. For definition of B_{ij} , see Eq. (a) in Introduction.

Atom	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
K(1)	0.3828(2)	0.7756(2)	0.6861(2)	2.10(6)	0.55(4)	3.02(8)	0.21(4)	-0.85(6)	-0.42(5)
K(2)	0.1106(1)	0.7023(3)	0.9322(2)	0.99(4)	1.08(5)	2.94(5)	0.35(4)	-0.03(5)	-0.16(5)
Sb(1)	0.24511(2)	0.25654(5)	0.75511(6)	0.26(1)	0.23(1)	0.23(1)	-0.01(1)	-0.02(1)	0.00(1)
Sb(2)	0.38308(2)	0.50765(5)	0	0.29(1)	0.16(1)	0.23(1)	0.01(1)	0.01(1)	-0.04(1)
Ge(1)	0.49751(5)	0.31733(7)	0.7498(1)	0.28(1)	0.27(1)	0.29(1)	0.00(1)	0.06(1)	0.00(2)
Ge(2)	0.18195(3)	0.51078(9)	0.5013(1)	0.45(1)	0.16(1)	0.35(1)	-0.00(1)	-0.00(2)	0.05(1)
O(1)	0.4804(4)	0.4959(7)	0.8690(4)	0.69(11)	0.53(14)	0.64(13)	-0.19(10)	0.35(10)	-0.29(11)
O(2)	0.9968(3)	0.9385(8)	0.1151(4)	0.60(12)	0.72(14)	0.38(11)	-0.08(10)	-0.07(9)	0.15(10)
O(3)	0.3888(3)	0.1674(6)	0.7400(5)	0.19(8)	0.44(11)	0.89(15)	-0.13(8)	0.04(9)	0.17(11)
O(4)	0.8987(3)	0.6600(7)	0.2718(5)	0.30(9)	0.56(12)	1.11(17)	0.01(8)	0.18(10)	0.16(13)
O(5)	0.1070(4)	0.3030(6)	0.4636(5)	0.71(12)	0.19(11)	1.02(16)	-0.15(9)	-0.48(11)	0.13(11)
O(6)	0.6026(4)	0.7866(7)	0.5350(5)	0.89(14)	0.09(11)	1.28(17)	-0.07(9)	0.18(12)	-0.13(11)
O(7)	0.2703(5)	0.5512(9)	0.3854(5)	0.64(13)	0.50(15)	0.76(14)	0.16(11)	0.26(12)	0.28(12)
O(8)	0.7648(5)	0.0370(9)	0.6272(5)	0.81(14)	0.58(15)	0.47(12)	0.29(12)	-0.14(11)	-0.35(11)
O(9) (OS1)	0.2246(5)	0.9693(9)	0.3789(5)	0.64(13)	0.64(15)	0.55(13)	-0.27(12)	0.39(20)	-0.44(12)
O(10) (OS2)	0.7178(5)	0.4533(9)	0.6312(5)	0.79(15)	0.68(15)	0.68(14)	-0.11(13)	-0.43(12)	0.38(13)

Table 35A-15-002. KSbOGeO₄. Bond lengths [Å] and bond angles [°] [91Bel].

M–O	O–O	O–M–O	M–O	O–O	O–M–O
Ge(1)-tetrahedron			Ge(2)-tetrahedron		
Ge(1)–O(1) 1.747(5)	O(1)–O(2) 2.752(6)	104.9(2)	Ge(2)–O(5) 1.740(4)	O(5)–O(6) 2.815(6)	108.1(2)
O(2) 1.724(5)	O(3) 2.880(7)	110.9(2)	O(6) 1.738(5)	O(7) 2.838(8)	109.7(3)
O(3) 1.749(4)	O(4) 2.883(7)	111.7(2)	O(7) 1.730(6)	O(8) 2.928(8)	113.0(3)
O(4) 1.737(4)	O(2)–O(3) 2.790(7)	106.9(2)	O(8) 1.770(6)	O(6)–O(7) 2.943(8)	116.1(3)
av. 1.739	O(4) 1.898(7)	113.7(2)	av. 1.744	O(8) 2.884(8)	110.6(3)
	O(3)–O(4) 2.831(5)	108.7(2)		O(7)–O(8) 2.667(8)	99.9(3)
Sb(1)-octahedron			Sb(2)-octahedron		
Sb(1)–O(3) 1.996(4)	O(3)–O(9) 2.907(3)	94.1(2)	Sb(2)–O(1) 1.964(5)	O(1)–O(2) 2.668(6)	85.7(2)
O(4) 1.988(4)	O(10) 2.667(7)	84.9(2)	O(2) 1.960(5)	O(9) 2.797(8)	91.4(2)
O(7) 1.960(6)	O(7) 2.732(8)	87.4(2)	O(5) 1.992(4)	O(5) 2.581(7)	81.5(2)
O(8) 1.954(6)	O(8) 2.822(8)	91.2(2)	O(6) 1.986(5)	O(6) 2.836(7)	91.8(2)
O(9) 1.976(6)	O(4)–O(9) 2.713(8)	86.4(2)	O(9) 1.946(6)	O(2)–O(5) 2.741(7)	87.8(2)
O(10) 1.956(6)	O(10) 2.900(8)	94.6(2)	O(10) 1.959(6)	O(10) 2.842(8)	93.0(2)
av. 1.972	O(7) 2.830(8)	91.6(2)	av. 1.968	O(6) 2.674(7)	85.3(2)
	O(8) 2.785(8)	89.9(2)		O(9)–O(5) 2.846(8)	92.5(2)
	O(9)–O(7) 2.825(9)	91.7(2)		O(10) 2.763(8)	90.0(3)
	O(8) 2.712(8)	87.3(2)		O(6) 2.876(8)	94.0(2)
	O(10)–O(7) 2.740(8)	88.8(3)		O(10)–O(5) 2.874(8)	93.3(2)
	O(8) 2.816(9)	92.2(3)		O(6) 2.869(8)	93.3(2)
K(1)-polyhedron			K(2)-polyhedron		
K(1)–O(2) 2.739(5)	K(1)–O(8) 2.662(6)		K(2)–O(1) 2.669(5)	K(2)–O(7) 2.834(7)	
O(3) 2.649(4)	O(1) 3.026(5)		O(4) 2.951(5)	O(2) 3.000(5)	
O(10) 2.882(7)	O(9) 3.225(6)		O(9) 2.729(6)	O(8) 3.174(6)	
O(5) 1.993(6)	O(6) 3.331(5)		O(5) 2.897(5)	O(10) 3.284(6)	
av. 2.938			av. 2.984	O(3) 3.319(6)	

Table 35A-15-003. KSbOGeO₄. Atomic coordinates and temperature parameters [\AA^2] [94Fav]. $T = 400\text{ }^\circ\text{C}$. For definition of U_{ij} , see Eq. (a) in Introduction.

Atom	x	y	z	Occup.	$B\text{ [}\text{\AA}^2\text{]}$
Sb(1)	0.13264(6)	0.250	0.750	1	0.76(1)
Sb(2)	0.000	0.000	0.000	1	0.784(9)
Ge(1)	0.250	0.0670(2)	0.000	1	0.90(2)
Ge(2)	0.9313(1)	0.250	0.250	1	0.98(2)
O(1)	0.2586(6)	0.226(1)	0.1270(7)	1	2.0(1)
O(2)	0.1436(5)	0.914(1)	1.0153(7)	1	1.5(1)
O(3)	0.8542(6)	0.044(1)	0.2848(7)	1	1.6(1)
O(4)	0.0158(6)	0.297(1)	0.3712(8)	1	1.8(1)
O(5)	0.9711(5)	0.713(1)	0.3764(7)	1	1.4(1)
K(1)	0.1324(7)	0.524(1)	0.0751(9)	0.364(8)	3.4(2)
K(2)	0.1378(5)	0.5469(9)	0.1520(8)	0.636(8)	5.3(2)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sb(1)	0.0100(3)	0.0097(2)	0.0092(2)	0	0	0.0021(4)
Sb(2)	0.0094(2)	0.0110(2)	0.0094(2)	−0.0011(3)	0.0008(3)	−0.0005(4)
Ge(1)	0.0102(5)	0.0121(5)	0.0118(5)	0	−0.0034(5)	0
Ge(2)	0.0138(5)	0.0102(5)	0.0133(5)	0	0	−0.0008(6)
O(1)	0.022(3)	0.024(3)	0.028(3)	0.012(3)	−0.011(3)	−0.015(3)
O(2)	0.013(3)	0.018(3)	0.028(3)	−0.004(3)	−0.007(3)	−0.006(3)
O(3)	0.019(3)	0.013(3)	0.027(3)	−0.001(3)	0.003(3)	−0.002(3)
O(4)	0.023(3)	0.020(3)	0.024(3)	0.007(3)	−0.007(3)	−0.013(3)
O(5)	0.019(3)	0.019(4)	0.016(3)	0.000(2)	−0.012(2)	0.006(3)
K(1)	0.047(4)	0.018(3)	0.063(5)	0.006(3)	0.006(5)	0.002(4)
K(2)	0.039(3)	0.033(2)	0.130(6)	0.007(2)	−0.004(4)	0.010(3)

Table 35A-15-004. KSbOGeO₄. Interatomic distances [Å] and angles [°] [94Fav]. *T* = 400 °C.

Sb(1)	O(1)	O(1)	O(3)	O(3)	O(5)	O(5)
O(1)	1.962(8)	2.66(2)	2.77(1)		3.91(1)	
O(1)	85.5(5)	1.962(8)	2.64(1)		2.82(1)	
O(3)		89.0(3)	1.990(7)	3.97(1)	2.87(1)	
O(3)		83.7(3)	170.0(5)	1.990(7)	2.91(1)	
O(5)		92.2(3)		93.1(3)	1.948(7)	2.68(2)
O(5)		176.7(3)		93.9(3)	90.3(5)	1.948(7)

Sb(2)	O(2)	O(2)	O(4)	O(4)	O(5)	O(5)
O(2)	1.991(7)	3.98(1)	2.83(1)		2.70(1)	
O(2)	180.0(0)	1.991(7)	2.73(1)		2.90(1)	
O(4)		92.0(3)	1.939(9)	3.88(2)	2.81(1)	
O(4)		88.0(3)	180.0(0)	1.939(9)	2.72(1)	
O(5)		85.8(3)		91.9(3)	1.973(8)	3.94(2)
O(5)		94.2(3)		88.0(3)	180.0(0)	1.973(8)

Ge(1)	O(1)	O(1)	O(2)	O(2)
O(1)	1.725(7)	2.74(2)		2.83(1)
O(1)	105.1(6)	1.725(7)		2.87(1)
O(2)		109.3(4)	1.742(6)	2.84(1)
O(2)		112.0(4)	109.2(5)	1.742(6)

Ge(2)	O(3)	O(3)	O(4)	O(4)
O(3)	1.742(8)	2.82(1)		2.87(1)
O(3)	108.3(5)	1.742(8)		2.91(1)
O(4)		110.8(4)	1.745(8)	2.68(2)
O(4)		113.3(4)	100.2(6)	1.745(8)