

**Table 35A-3-001.** AgSbOSiO<sub>4</sub>. Atomic coordinates and anisotropic temperature parameters [94Bel].  $f$ : occupancy ratio. For definition of anisotropic temperature parameters  $B_{ij}$ , see Eq. (a) in Introduction.

Atom	$f$	$x$	$y$	$z$	$B_{11}$	$B_{22}$	$B_{33}$	$B_{12}$	$B_{13}$	$B_{23}$
Ag(1)	0.45	0.3905(4)	0.8003(7)	0.3561(5)	4.0(2)	2.1(2)	5.1(3)	1.8(2)	−0.9(2)	0.0(2)
Ag(1')	0.47	0.3610(4)	0.7757(8)	0.2954(6)	5.4(2)	2.6(2)	4.6(2)	0.2(2)	1.8(2)	−0.3(2)
Ag(2)	0.35	0.1074(5)	0.7100(10)	0.0921(6)	4.0(3)	5.7(3)	4.8(4)	3.3(3)	−1.7(3)	−1.4(3)
Ag(2')	0.61	0.1178(2)	0.7187(5)	0.1484(4)	2.1(1)	2.0(1)	6.6(2)	0.4(1)	0.5(1)	1.0(1)
Ag(3)	0.01	0.255	0.247	0.750	8(2)					
Ag(4)	0.04	0.084(4)	0.565(8)	0.007(6)	7(2)	3(2)	5(2)	2(1)	1(2)	−6(3)
Ag(5)	0.07	0.013(3)	0.660(6)	0.267(7)	8(2)	1.4(6)	7(2)	−0(1)	−4(1)	2(1)
Sb(1)	1	0.2463(1)	0.2573(3)	0.2484(2)	0.28(2)	1.11(3)	0.30(2)	−0.04(3)	0.09(3)	−0.20(3)
Sb(2)	1	0.3830(1)	0.5075(3)	0	0.48(2)	0.60(3)	0.24(2)	−0.05(6)	−0.02(7)	0.01(3)
Si(1)	1	0.4956(6)	0.3289(8)	0.256(1)	0.2(1)	0.9(2)	0.1(1)	0.4(2)	0.1(2)	0.3(2)
Si(2)	1	0.1876(4)	0.506(2)	0.499(1)	0.6(1)	0.7(2)	0.4(1)	−0.0(3)	−0.0(4)	0.0(2)
O(1)	1	0.495	0.490	0.130	1.5(7)	3.2(7)	1.2(7)	−0.2(8)	−1.7(6)	0.9(7)
O(2)	1	0.506	0.487	0.371	0.8(4)	1.0(5)	0.8(4)	0.4(6)	0.2(4)	−0.8(5)
O(3)	1	0.392	0.188	0.261	0.3(1)	1.2(6)	0.1(1)	−0.2(1)	0.4(3)	−0.2(1)
O(4)	1	0.594(1)	0.167(2)	0.245(1)	0.3(3)	1.2(5)	1.0(5)	−0.2(4)	−0.1(3)	0.6(6)
O(5)	1	0.112(1)	0.310(2)	0.537(1)	0.9(5)	1.1(5)	0.4(5)	0.3(3)	1.3(5)	−0.4(4)
O(6)	1	0.108(1)	0.706(2)	0.481(1)	1.4(6)	0.6(4)	0.1(1)	0.1(1)	0.1(1)	0.2(1)
O(7)	1	0.269(1)	0.546(2)	0.615(1)	0.1(5)	1.3(5)	0.5(5)	0.4(4)	−0.5(4)	0.2(4)
O(8)	1	0.262(1)	0.469(2)	0.380(1)	0.4(5)	2.0(6)	0.4(5)	−0.8(5)	0.3(4)	−0.4(4)
O(9)	1	0.271(1)	0.492(3)	0.129(1)	1.1(5)	1.3(5)	0.5(5)	−0.1(6)	0.1(4)	−0.4(6)
O(10)	1	0.222(1)	0.031(2)	0.370(1)	0.3(4)	0.3(5)	0.6(4)	0.6(4)	0.3(4)	0.4(4)

**Table 35A-3-002.** AgSbOSiO<sub>4</sub>. Interatomic distances [Å] [94Bel].

Si(1)-tetrahedron				Si(2)-tetrahedron			
Si(1)–O(1)	1.69(1)	O(1)–O(2)	2.59(2)	Si(2)–O(5)	1.62(2)	O(5)–O(6)	2.58(2)
O(2)	1.59(1)	O(3)	2.71(1)	O(6)	1.64(2)	O(7)	2.64(2)
O(3)	1.60(1)	O(4)	2.71(1)	O(7)	1.65(2)	O(8)	2.74(2)
O(4)	1.63(1)	O(2)–O(3)	2.66(1)	O(8)	1.63(2)	O(6)–O(7)	2.72(2)
(Si–O) <sub>av</sub>	1.63	O(4)	2.68(1)	(Si–O) <sub>av</sub>	1.63	O(8)	2.70(2)
		O(3)–O(4)	2.60(1)			O(7)–O(8)	2.57(2)
Sb(1)-octahedron				Sb(2)-octahedron			
Sb(1)–O(3)	1.93(1)	O(3)–O(7)	2.75(1)	Sb(2)–O(1)	2.00(1)	O(1)–O(2)	2.79(1)
O(4)	2.01(1)	O(8)	2.75(1)	O(2)	1.98(1)	O(5)	2.64(2)
O(7)	1.97(1)	O(9)	2.86(2)	O(5)	1.96(1)	O(6)	2.74(2)
O(8)	1.96(1)	O(10)	2.67(1)	O(6)	1.93(1)	O(9)	2.86(2)
O(9)	1.99(2)	O(4)–O(7)	2.89(2)	O(9)	2.00(1)	O(10)–O(5)	2.88(2)
O(10)	1.96(1)	O(8)	2.73(2)	O(10)	1.95(1)	O(6)	2.79(2)
(Sb–O) <sub>av</sub>	1.97	O(9)	2.77(2)	(Sb–O) <sub>av</sub>	1.97	O(2)	2.77(1)
		O(10)	2.85(1)			O(9)	2.80(2)
		O(7)–O(9)	2.88(2)			O(2)–O(5)	2.93(2)
		O(10)	2.73(2)			O(6)	2.62(1)
		O(8)–O(9)	2.70(2)			O(9)–O(5)	2.70(2)
		O(10)	2.82(2)			O(6)	2.88(2)
Ag(1)-polyhedron		Ag(2)-polyhedron		Ag(3)-polyhedron			
Ag(1)–O(2)	2.48(1)	Ag(2)–O(1)	2.43(1)	Ag(3)–O(9)	2.10(2)	Ag(3)–Ag(1)	2.21(7)
O(3)	2.66(1)	O(9)	2.54(2)	O(10)	2.23(1)	Ag(1')	1.57(6)
O(10)	2.61(1)	O(7)	2.66(2)	O(8)	2.26(1)	Ag(2)	2.46(7)
O(8)	2.68(2)	O(5)	2.89(2)	O(7)	2.39(1)	Ag(2')	1.98(6)
		O(4)	2.90(1)	O(5)	2.96(2)		
				O(6)	3.05(1)		
Ag(1')-polyhedron		Ag(2')-polyhedron					
Ag(1')–O(8)	2.49(2)	Ag(2')–O(9)	2.44(2)				
O(10)	2.53(1)	O(1)	2.44(2)				
O(3)	2.67(1)	O(7)	2.56(1)				
O(2)	2.73(1)	O(4)	2.67(1)				
O(9)	2.78(2)	Ag(2)–Ag(2')	0.62(1)				
O(5)	2.80(2)	Ag(2)–Ag(1)	3.62				
Ag(1)–Ag(1')	0.77(1)	Ag(2')–Ag(1')	4.72				
Ag(4)-polyhedron		Ag(5)-polyhedron					
Ag(4)–O(3)	2.76(7)	Ag(5)–O(4)	2.33(4)				
O(5)	2.70(5)	O(2)	2.49(5)				
O(9)	2.73(6)	O(6)	2.61(7)				
O(10)	2.86(6)	O(1)	2.67(5)				
O(4)	2.95(7)	O(3)	2.70(4)				
O(6)	3.05(5)	O(5)	2.96(7)				
Ag(4)–Ag(1)	2.35(6)	Ag(5)–Ag(1)	1.85(5)				
Ag(1')	2.99(6)	Ag(1')	2.01(5)				
Ag(2)	1.32(6)	Ag(2)	2.26(7)				
Ag(2')	1.84(7)	Ag(2')	1.89(6)				
Ag(3)	3.49(9)	Ag(3)	3.04(5)				
		Ag(4)	3.01(9)				