Table 35A-19-001. $TlSbOGeO_4$. Atomic positions and anisotropic temperature parameters [92Bel]. For definition of B_{ij}, see Eq. (a) in Introduction.

Atom	Occup.	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Tl(1)	0.35	–0.1377(5)	0.0335(8)	0.3966(4)	1.89(14)	1.08(10)	4.8(2)	–0.3(1)	0.7(2)	–0.8(2)
Tl(2)	0.65	–0.1422(2)	0.4556(4)	0.1548(2)	1.36(6)	1.63(6)	3.7(1)	0.25(6)	–0.16(10)	–0.63(9)
Sb(1)	1	0.1307(1)	0.25	0.25	0.40(6)	0.38(4)	0.37(5)	0	0	–0.11(6)
Sb(2)	1	0	0	0	0.45(5)	0.47(4)	0.29(4)	–0.00(4)	–0.04(7)	0.05(6)
Ge(1)	1	0.25	0.0667(4)	0	0.42(8)	0.49(7)	0.62(9)	0	0.05(11)	0
Ge(2)	1	0.0681(2)	0.75	0.25	0.59(9)	0.32(7)	0.54(9)	0	0	–0.01(9)
O(1)	1	–0.1435(9)	0.0844(18)	0.0148(13)	0.1(4)	1.3(4)	1.7(6)	0.1(4)	–0.3(4)	–0.5(4)
O(2)	1	0.0189(9)	0.2024(19)	–0.1303(12)	0.9(5)	1.5(5)	0.1(3)	–0.4(4)	–0.0(4)	0.6(3)
O(3)	1	–0.0267(9)	–0.2096(18)	–0.1225(16)	0.5(4)	0.7(4)	1.8(7)	–0.4(4)	–0.2(5)	–0.2(4)
O(4)	1	–0.1411(11)	0.0413(19)	–0.2875(12)	1.6(5)	1.0(4)	1.3(4)	0.9(5)	–0.8(5)	0.5(4)
O(5)	1	–0.2412(9)	–0.2253(21)	–0.1271(14)	0.1(4)	2.0(5)	2.3(6)	–0.7(4)	0.4(5)	–0.6(5)

Table 35A-19-002. $TlSbOGeO_4$. Coordinates of the cations [$\cdot 10^{-4}$] and oxygens [$\cdot 10^{-3}$] and their anisotropic temperature parameters. U_{ij} [$\cdot 10^{-3}$ Å^2] [94Bel]. T = 280 K and T = 253 K. For definition of U_{ij}, see Eq. (d) in Introduction.

Atom	Occup.	x	y	z	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
				T = 280 K						
Tl	0.65	–1418(2)	4552(4)	1541(2)	24(1)	29(1)	43(1)	–6(1)	–3(1)	4(1)
Tl′	0.35	–1380(4)	4679(7)	1059(5)	34(2)	22(1)	60(3)	–12(2)	–14(2)	5(1)
Sb(1)	1	1307(1)	2500	2500	10(1)	12(1)	6(1)	–1(1)	0	0
Sb(2)	1	0	0	0	11(1)	13(1)	5(1)	1(1)	0(1)	–1(1)
Ge(1)	1	2500	668(3)	0	11(1)	15(1)	7(1)	0	2(1)	0
Ge(2)	1	682(2)	7500	2500	14(1)	11(1)	7(1)	1(1)	0	0
O(1)	1	–144(1)	81(2)	14(1)	13(3)	18(4)	10(4)	–7(4)	4(3)	0(3)
O(2)	1	18(1)	201(2)	–134(1)	16(4)	22(4)	17(5)	10(4)	–3(4)	0(3)
O(3)	1	–28(1)	–208(2)	–124(1)	18(4)	14(4)	6(4)	–4(3)	–4(3)	3(3)
O(4)	1	–142(1)	42(1)	–287(1)	25(4)	17(4)	16(4)	–5(4)	–4(4)	–5(4)
O(5)	1	–240(1)	–224(2)	–129(1)	21(4)	28(5)	17(5)	–6(4)	7(4)	3(4)
				T = 253 K						
Tl(1)	0.6	3878(2)	7843(3)	6464(3)	27(1)	20(1)	57(1)	–7(1)	–6(1)	2(1)
Tl(1)′	0.4	3917(3)	7943(5)	5938(3)	20(1)	23(1)	29(1)	2(1)	3(1)	6(1)
Tl(2)	1	1077(1)	7065(3)	9015(2)	27(1)	31(1)	74(1)	–14(1)	–7(1)	3(1)
Sb(1)	1	2473(2)	2522(4)	7520(2)	13(1)	15(1)	11(1)	0(1)	0(1)	–1(1)
Sb(2)	1	3805(1)	5025(3)	0	13(1)	14(1)	12(1)	–2(1)	0(1)	–2(1)
Ge(1)	1	4972(3)	3167(3)	7498(4)	14(1)	17(1)	12(1)	1(1)	0(1)	–2(1)
Ge(2)	1	1818(1)	5060(5)	4996(4)	15(1)	14(1)	12(1)	1(1)	4(1)	1(1)
O(1)	1	485(1)	491(2)	875(1)	13(3)*)					
O(2)	1	995(1)	955(2)	117(1)	13(2)					
O(3)	1	386(1)	167(2)	744(1)	11(2)					
O(4)	1	901(2)	664(3)	274(2)	20(4)					
O(5)	1	111(1)	298(2)	456(1)	7(2)					
O(6)	1	605(2)	784(3)	525(2)	19(4)					
O(7)	1	271(1)	557(2)	388(1)	9(2)					
O(8)	1	765(2)	33(3)	631(2)	27(4)					
O(9)	1	222(2)	952(3)	377(2)	21(3)					
O(10)	1	718(1)	466(2)	630(1)	14(2)					

*) Below this line, isotropic temperature parameters were used.

Table 35A-19-003. $TlSbOGeO_4$. Interatomic distances [Å] [94Bel]. T = 280 K and T = 253 K.

T = 280 K

Ge(1)-tetrahedron				Ge(2)-tetrahedron			
Ge(1)–O(1) × 2*)	1.730(11)	O(1)–O(1)	2.84(2)	Ge(2)–O(2) × 2	1.721(14)	O(2)–O(2)′	0.57(1)
O(5) × 2	1.744(15)	O(5)–O(5)′	2.79(1)	O(4) × 2	1.744(11)	O(4)–O(4)′	2.89(1)
av.	1.739	O(1)–O(5) × 2	2.85(1)	av.	1.732	O(2)–O(4)′ × 2	2.88(2)
		O(1)–O(5)′ × 2	2.84(2)			O(4)–O(2)′ × 2	2.86(2)
Sb(1)-octahedron				Sb(2)-octahedron			
Sb(1)–O(3) × 2	1.940(12)	O(3)–O(3)′	2.76(1)	Sb(2)–O(1) × 2	1.999(11)	O(1)–O(2) × 2	2.80(2)
O(4) × 2	1.986(8)	O(4) × 2	2.85(1)	O(2) × 2	1.981(14)	O(2)′ × 2	2.83(2)
O(5) × 2	1.955(14)	O(5) × 2	2.82(2)	O(3) × 2	1.958(12)	O(3) × 2	2.88(2)
av.	1.960	O(4)–O(3)′ × 2	2.85(2)	av.	1.980	O(3)′ × 2	2.72(2)
		O(5) × 2	2.77(2)			O(2)–O(3) × 2	2.79(2)
		O(5)′ × 2	2.64(2)			O(3)′ × 2	2.78(2)
		O(5)–O(5)′	2.62(2)				
Tl-polyhedron				Tl′-polyhedron			
Tl–O(1)	2.91(1)	Tl–O(4)	2.96(2)	Tl′–O(1)	2.76(1)	Tl′–O(4)	3.16(2)
O(2)	2.83(1)	O(5)	2.67(1)	O(2)	2.74(1)	O(4)′	3.16(2)
O(2)′	3.25(1)	O(5)′	3.33(2)	O(3)	2.82(1)	O(5)	2.63(2)
O(3)	2.82(1)			Tl–Tl′	0.527(6)		

T = 253 K

Ge(1)-tetrahedron				Ge(2)-tetrahedron			
Ge(1)–O(1)	1.79(2)	O(1)–O(2)	2.81(2)	Ge(2)–O(5)	1.74(2)	O(5)–O(6)	2.88(2)
O(2)	1.71(2)	O(3)	2.90(2)	O(6)	1.75(2)	O(7)	2.85(2)
O(3)	1.79(2)	O(4)	2.88(2)	O(7)	1.72(2)	O(8)	3.00(2)
O(4)	1.72(2)	O(2)–O(3)	2.85(2)	O(8)	1.82(2)	O(6)–O(7)	2.86(2)
av.	1.75	O(4)	2.87(2)	av.	1.76	O(8)	2.93(2)
		O(3)–O(4)	2.86(2)			O(7)–O(8)	2.68(2)
Sb(1)-octahedron				Sb(2)-octahedron			
Sb(1)–O(3)	1.95(2)	O(3)–O(7)	2.72(2)	Sb(2)–O(1)	1.93(2)	O(1)–O(2)	2.62(2)
O(4)	2.07(2)	O(8)	2.85(2)	O(2)	2.00(2)	O(5)	2.57(3)
O(7)	1.98(2)	O(9)	2.79(2)	O(5)	2.03(2)	O(6)	2.72(2)
O(8)	1.95(2)	O(10)	2.71(2)	O(6)	1.94(2)	O(9)	2.78(2)
O(9)	1.94(2)	O(4)–O(7)	2.82(2)	O(9)	1.94(2)	O(10)–O(5)	2.79(2)
O(10)	2.00(2)	O(8)	2.84(2)	O(10)	1.94(1)	O(6)	2.84(2)
av.	1.98	O(9)	2.74(2)	av.	1.96	O(2)	2.85(2)
		O(10)	2.99(2)			O(9)	2.78(2)
		O(7)–O(9)	2.71(2)			O(2)–O(5)	2.80(2)
		O(10)	2.79(2)			O(6)	2.75(2)
		O(8)–O(9)	2.66(2)			O(9)–O(5)	2.88(2)
		O(10)	2.95(2)			O(6)	2.73(2)

Tl(1)-polyhedron		Tl(1)′-polyhedron		Tl(2)-polyhedron	
Tl(1)–O(1)	3.40(2)	Tl(1)′–O(1)	3.45(2)	Tl(2)–O(1)	2.62(2)
O(2)	2.72(2)	O(2)	2.73(2)	O(2)	3.22(2)
O(3)	2.76(2)	O(3)	2.96(2)	O(4)	2.83(2)
O(5)	3.34(1)	O(6)	2.95(2)	O(5)	2.98(2)
O(6)	3.18(2)	O(7)	3.16(2)	O(7)	2.85(2)
O(8)	2.68(2)	O(8)	2.79(2)	O(8)	3.46(2)
O(10)	2.82(2)	O(10)	2.84(2)	O(9)	2.85(2)
Tl(1)–Tl(1)′	0.573(5)				

*) The numbers of symmetrically equivalent distances.

Table 35A-19-004. $TlSbOGeO_4$. Bond lengths [Å] and bond angles [°] [92Bel].

M–O		O–O		O–M–O	
		Ge1-tetrahedron			
Ge–O1 × 2 *)	1.750(12)	O1–O1′	2.86(2)		109.7(6)
O5 × 2	1.732(15)	O5–O5′	2.74(2)		104.8(6)
av.	1.741	O1–O5 × 2	2.88(2)	× 2	111.6(6)
		O1–O5′ × 2	2.84(2)	× 2	109.6(6)
		Ge2-tetrahedron			
Ge2–O2 × 2	1.763(13)	O2–O2′	2.65(2)		97.5(6)
O4 × 2	1.746(13)	O4–O4′	2.90(2)		112.1(6)
av.	1.755	O2–O4′ × 2	2.88(2)	× 2	110.0(6)
		O4–O2′ × 2	2.93(2)	× 2	113.2(6)
		Sb1-octahedron			
Sb1–O3 × 2	1.970(15)	O3–O3′	2.80(2)		90.4(5)
O4 × 2	1.988(13)	O4 × 2	2.88(2)	× 2	92.3(6)
O5 × 2	1.988(14)	O5 × 2	2.87(2)	× 2	92.8(6)
av.	1.982	O4–O3′ × 2	2.86(2)	× 2	92.4(6)
		O5 × 2	2.82(2)	× 2	90.1(6)
		O5′ × 2	2.66(2)	× 2	83.9(6)
		O5–O5′	2.66(2)		84.2(6)
		Sb2-octahedron			
Sb2–O1 × 2	2.003(12)	O1–O2 × 2	2.78(2)	× 2	89.2(5)
O2 × 2	1.952(13)	O2′ × 2	2.82(2)	× 2	90.8(5)
O3 × 2	1.954(14)	O3′ × 2	2.91(2)	× 2	94.6(6)
av.	1.973	O3	2.68(2)	× 2	85.4(6)
		O2–O3 × 2	2.82(2)	× 2	91.9(6)
		O3′ × 2	2.72(2)	× 2	88.1(6)

M–O

Tl1-polyhedron				Tl2-polyhedron			
Tl1–O5	2.627(14)	Tl1–O4	3.179(15)	Tl2–O5	2.653(14)	Tl12–O2′	3.280(13)
O1	2.720(13)	O4′	3.398(14)	O3	2.811(13)	O5	3.341(15)
O2	2.734(14)	O5′	3.502(15)	O2	2.825(13)	O3	3.470(15)
O3	2.793(14)	O3′	3.572(15)	O1	2.897(13)	O1′	3.563(14)
		av.	3.066	O4	2.960(15)	av.	3.089

*) The numbers of symmetrically equivalent distances and angles.