

**Table 35A-1-001.** NaSbOSiO<sub>4</sub>, AgSbOSiO<sub>4</sub>, KSbOSiO<sub>4</sub>, NaSbOGeO<sub>4</sub>, KSbOGeO<sub>4</sub>, AgSbOGeO<sub>4</sub>. Conditions for synthesis and some characteristics [93Mil2].  $T_{\text{salt}}$ : temperature of the molten salt.  $I_{2\omega}/I_{\omega}(\text{SiO}_2)$ : SHG power compared to that of SiO<sub>2</sub>.

Compound	Substrate	Molten salt	$T_{\text{salt}}$ [°C]	$a$ [Å]	$b$ [Å]	$c$ [Å]	$V$ [Å <sup>3</sup> ]	Decomposition temperature [°C]	$I_{2\omega}/I_{\omega}(\text{SiO}_2)$ 20 °C	$\theta \pm 30 \text{ K}$	Color
NaSbOSiO <sub>4</sub>	KSbOSiO <sub>4</sub>	NaNO <sub>3</sub>	350	12.825(7)	6.326(3)	10.614(6)	861.04	1150–1200	0.4	730	white
AgSbOSiO <sub>4</sub>	NaSbOSiO <sub>4</sub>	AgNO <sub>3</sub>	250	12.815(6)	6.356(3)	10.716(5)	872.84	900–950	1.1	430	yellow
AgSbOSiO <sub>4</sub>	KSbOSiO <sub>4</sub>	AgNO <sub>3</sub>	250	12.789(7)	6.333(3)	10.729(6)	869.00	900–950	1.1	430	flesh colored
NaSbOGeO <sub>4</sub>	KSbOGeO <sub>4</sub>	NaNO <sub>3</sub>	350	12.989(5)	6.439(2)	10.685(4)	893.65	800–900	0.8	>900	white
AgSbOGeO <sub>4</sub>	KSbOGeO <sub>4</sub>	AgNO <sub>3</sub>	250	12.97(1)	6.426(5)	10.69(1)	891.33	700–800	1.5	440	greenish yellow
NaSbOSiO <sub>4</sub>	solid phase synthesis			12.800(4)	6.321(2)	10.618(3)	859.13	1150–1200	0.4	700	white
KSbOSiO <sub>4</sub>				13.036(5)	6.488(2)	10.624(4)	898.65	>1300	0.5	330	white
KSbOGeO <sub>4</sub>				13.231(5)	6.600(2)	10.759(4)	939.56	>1250	0.95	330	white

**Table 35A-1-002.** NaSbOSiO<sub>4</sub>. Atomic coordinates and temperature parameters [94Fav].  $T = 570\text{ }^{\circ}\text{C}$  (paraelectric phase).  $B$ : isotropic temperature parameter defined in Eq. (e) in Introduction.  $U_{ij}$ : anisotropic temperature parameter defined in Eq. (a) in Introduction.

(a)	$x$	$y$	$z$	Occupancy	$B\text{ [}\text{\AA}^2\text{]}$
Sb(1)	0.13257(5)	0.250	0.750	1	0.908(6)
Sb(2)	0.000	0.000	0.000	1	0.949(6)
Si(1)	0.250	0.0774(4)	0.000	1	1.09(4)
Si(2)	0.9336(2)	0.250	0.250	1	1.11(4)
O(1)	0.2585(5)	0.232(1)	0.1215(5)	1	2.07(9)
O(2)	0.1500(4)	0.9257(9)	1.0144(6)	1	1.70(9)
O(3)	0.8574(5)	0.0523(8)	0.2770(5)	1	1.8(1)
O(4)	0.0122(5)	0.287(1)	0.3676(5)	1	2.3(1)
O(5)	0.9760(5)	0.7257(9)	0.3791(5)	1	1.79(9)
Na(1)	0.120(1)	0.521(2)	0.066(2)	0.57(1)	8.4(4)
Na(2)	0.142(1)	0.539(4)	0.163(2)	0.43(1)	8.6(6)

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{12}$	$U_{13}$	$U_{23}$
Sb(1)	0.0148(2)	0.0106(2)	0.0091(2)	0	0	0.0014(2)
Sb(2)	0.0138(2)	0.0134(2)	0.0090(1)	−0.0014(2)	0.0015(2)	−0.0013(2)
Si(1)	0.0132(9)	0.016(1)	0.0124(9)	0	−0.003(1)	0
Si(2)	0.016(1)	0.0134(9)	0.0123(8)	0	0	−0.002(1)
O(1)	0.026(2)	0.032(3)	0.021(2)	−0.000(3)	−0.009(2)	−0.013(2)
O(2)	0.018(2)	0.024(2)	0.023(2)	−0.003(2)	−0.002(2)	0.003(2)
O(3)	0.030(3)	0.012(2)	0.028(3)	−0.005(2)	0.006(2)	−0.002(2)
O(4)	0.035(3)	0.036(3)	0.017(2)	0.013(3)	−0.009(2)	−0.011(2)
O(5)	0.031(2)	0.016(2)	0.021(2)	−0.007(2)	−0.012(2)	0.005(2)
Na(1)	0.106(8)	0.050(6)	0.16(1)	0.019(7)	0.063(9)	0.002(9)
Na(2)	0.07(1)	0.10(1)	0.16(2)	0.00(1)	0.02(1)	0.03(2)