

TABLE 5a. Interatomic distances (Å) of the tok\_2 and tok\_3 crystals.

	tok_2	tok_3		tok_2	tok_3
Tetrahedra					
Si1–O2	1.591(3)	1.594(4)	Si2–O5	1.584(3)	1.583(4)
Si1–O3	1.602(3)	1.604(3)	Si2–O6	1.605(3)	1.597(3)
Si1–O4	1.625(3)	1.631(4)	Si2–O4	1.629(3)	1.632(3)
Si1–O1	1.647(3)	1.645(3)	Si2–O7	1.647(3)	1.646(3)
<Si1–O>	1.616(6)	1.619(7)	<Si2–O>	1.616(6)	1.615(7)
Si3–O8	1.577(3)	1.575(4)	Si4–O12	1.576(3)	1.577(3)
Si3–O9	1.639(3)	1.635(3)	Si4–O13	1.636(3)	1.643(3)
Si3–O7	1.641(3)	1.636(3)	Si4–O10	1.653(3)	1.638(4)
Si3–O1	1.635(3)	1.633(3)	Si4–O11	1.641(3)	1.639(4)
<Si3–O>	1.623(6)	1.620(7)	<Si4–O>	1.627(6)	1.624(7)
Si5–O14	1.578(3)	1.577(3)	Si6–O17	1.575(3)	1.580(3)
Si5–O15	1.634(3)	1.638(4)	Si6–O9	1.624(3)	1.625(3)
Si5–O16	1.649(3)	1.648(3)	Si6–O10	1.640(3)	1.644(3)
Si5–O13	1.648(3)	1.651(3)	Si6–O16	1.651(3)	1.647(3)
<Si5–O>	1.627(6)	1.629(7)	<Si6–O>	1.623(6)	1.624(6)
Si7–O19	1.589(3)	1.597(4)			
Si7–O18	1.636(4)	1.633(4)			
Si7–O11	1.640(3)	1.642(3)			
Si7–O15	1.639(3)	1.632(4)			
<Si7–O>	1.626(7)	1.626(8)			
6-, 7-Coordinate polyhedra					
M1 <sub>(Ca)</sub> –O5	2.103(3)	2.088(4)	M1 <sub>(Ti)</sub> –O20	1.822(9)	1.873(8)
M1 <sub>(Ca)</sub> –O2	2.099(3)	2.092(4)	M1 <sub>(Ti)</sub> –O20	2.01(1)	2.045(9)
M1 <sub>(Ca)</sub> –O12	2.127(3)	2.118(4)	M1 <sub>(Ti)</sub> –O2	2.10(1)	2.078(9)
M1 <sub>(Ca)</sub> –O20	2.190(4)	2.192(4)	M1 <sub>(Ti)</sub> –O5	2.321(9)	2.275(9)
M1 <sub>(Ca)</sub> –O20	2.249(4)	2.261(4)	M1 <sub>(Ti)</sub> –O19	2.40(1)	2.378(9)
M1 <sub>(Ca)</sub> –O19	2.347(4)	2.335(4)	M1 <sub>(Ti)</sub> –O12	2.483(9)	2.424(8)
<M1 <sub>(Ca)</sub> –O>	2.186(9)	2.18(1)	<M1 <sub>(Ti)</sub> –O>	2.19(2)	2.18(2)
M2–O14	2.299(3)	2.287(4)	M3–O12	2.327(3)	2.323(4)
M2–O20	2.351(3)	2.354(4)	M3–O17	2.344(3)	2.341(3)
M2–O19	2.356(3)	2.341(4)	M3–O3	2.363(3)	2.367(3)
M2–O5	2.409(3)	2.408(4)	M3–O6	2.371(3)	2.379(3)
M2–O2	2.420(3)	2.422(4)	M3–O8	2.376(3)	2.375(3)
M2–O19	2.489(3)	2.480(4)	M3–O3	2.417(3)	2.411(3)
M2–O4	2.839(4)	2.835(5)	<M3–O>	2.366(7)	2.366(8)
<M2–O>	2.452(8)	2.45(1)			
M4–O14	2.300(3)	2.302(4)			
M4–O17	2.337(3)	2.334(3)			
M4–O8	2.348(3)	2.351(3)			
M4–O6	2.385(3)	2.390(3)			
M4–O6	2.418(3)	2.414(3)			
M4–O3	2.420(3)	2.412(3)			
<M4–O>	2.368(6)	2.367(8)			
K sites					
K1–O20			K10–O20	2.701(6)	2.696(6)
K1–O11			K10–O5	2.986(4)	2.982(5)
K1–O15			K10–O2	2.992(7)	3.002(6)
K1–O5			K10–O7	3.137(6)	3.141(6)
K1–O7			K10–O15	3.243(7)	3.227(6)
K1–O13			K10–O1	3.257(7)	3.256(6)
K1–O2			K10–O11	3.339(6)	3.324(6)
<K1–O>			<K10–O>	3.09(2)	3.09(2)

(continued)

TABLE 5a. (contd.)

	tok_2	tok_3		tok_2	tok_3
K11-O20	2.82(2)	2.84(2)	K12-O20	2.79(3)	2.84(3)
K11-O15	2.94(2)	2.95(2)	K12-O2	3.03(3)	3.04(3)
K11-O11	3.03(2)	3.06(2)	K12-O11	3.09(3)	3.06(3)
K11-O13	3.31(2)	3.34(2)	K12-O1	3.26(3)	3.22(3)
K11-O11	3.38(2)	3.39(2)	K12-O10	3.27(2)	3.32(2)
K11-O15	3.42(2)	3.41(2)	K12-O5	3.34(3)	3.32(2)
K11-O2	3.44(2)	3.42(2)	K12-O7	3.34(3)	3.33(3)
K11-O5	3.45(2)	3.43(2)	K12-O18	3.37(3)	3.35(3)
K11-O18	3.47(2)	3.44(2)	K12-O15	3.41(3)	3.39(3)
K11-O16	3.47(2)	3.47(2)	<K12-O>	3.21(9)	3.21(8)
K11-O10	3.51(2)	3.49(2)			
<K11-O> <sub>10</sub>	3.27(6)	3.28(6)			
<K11-O> <sub>11</sub>	3.29(6)	3.29(6)			
K2-O9	2.762(3)	2.768(3)			
K2-O1	2.800(3)	2.808(3)			
K2-O4	2.854(3)	2.856(4)			
K2-O7	2.858(3)	2.859(4)			
K2-O16	2.861(4)	2.867(4)			
K2-O10	2.886(3)	2.884(3)			
K2-O13	2.980(3)	2.976(4)			
K2-O18	3.213(4)	3.204(4)			
K2-O8	3.281(3)	3.280(3)			
K2-O17	3.372(3)	3.369(4)			
<K2-O> <sub>9</sub>	2.94(1)	2.95(1)			
<K2-O> <sub>10</sub>	2.99(1)	2.99(1)			

\*R. *et al.* (1989)= Rozhdestvenskaya *et al.* (1989).