

**Table 35B-2-001.** Cs<sub>0.6</sub>K<sub>0.4</sub>TiOAsO<sub>4</sub>. Atomic coordinates and temperature parameters [94Nor]. *B*: isotropic temperature parameters. For definition of *B*, see Eq. (e) in Introduction.

<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i>		
(a) 20 °C				(c) 400 °C					
Cs1	0.3816(1)	0.7773(2)	0.6661(3)	3.34(8)	Cs1	0.3872(2)	0.7880(3)	0.6327(6)	7.2(2)
Cs2	0.1054(1)	0.6778(1)	0.9126(2)	1.59(3)	Cs2	0.1083(1)	0.6933(3)	0.8936(4)	4.9(1)
Ti1	0.3730(1)	0.4886(2)	0.0000	0.66(5)	Ti1	0.3724(1)	0.4955(4)	0.00000	1.40(7)
Ti2	0.2548(1)	0.2570(3)	0.7435(3)	0.65(5)	Ti2	0.2448(2)	0.7594(4)	0.2450(5)	1.35(7)
As1	0.5033(1)	0.3279(1)	0.7400(2)	0.61(3)	As1	0.5034(1)	0.3267(2)	0.7430(4)	1.26(4)
As2	0.3184(1)	0.9907(1)	0.9868(2)	0.61(3)	As2	0.3210(1)	0.9937(2)	0.9887(3)	1.30(4)
O1	0.4883(6)	0.4704(13)	0.8651(8)	1.3(3)	O1	0.4886(10)	0.469(3)	0.867(1)	2.8(6)
O2	0.5144(6)	0.4757(14)	0.6135(8)	1.5(3)	O2	0.5166(11)	0.473(2)	0.618(1)	2.7(5)
O3	0.4033(5)	0.1803(12)	0.7125(7)	1.1(2)	O3	0.4019(9)	0.187(2)	0.714(2)	2.8(6)
O4	0.1069(5)	0.3143(11)	0.7527(7)	1.0(2)	O4	0.1051(9)	0.319(2)	0.760(1)	2.0(5)
O5	0.3866(5)	0.7881(9)	0.9517(7)	0.9(2)	O5	0.3892(10)	0.794(2)	0.952(1)	2.5(5)
O6	0.6096(6)	0.8109(11)	0.5201(8)	1.3(3)	O6	0.6119(10)	0.803(2)	0.527(2)	2.9(6)
O7	0.2474(6)	0.0330(11)	0.8596(7)	1.0(2)	O7	0.2506(9)	0.039(2)	0.860(1)	2.5(5)
O8	0.2641(6)	0.4461(13)	0.6007(8)	1.2(3)	O8	0.2611(9)	0.447(2)	0.603(1)	2.1(4)
OT1	0.2207(5)	0.0388(12)	0.6050(7)	1.0(2)	OT1	0.2202(9)	0.045(2)	0.607(1)	1.9(4)
OT2	0.2865(5)	0.4353(11)	0.8549(8)	1.0(2)	OT2	0.2856(8)	0.437(2)	0.857(1)	2.1(4)
(b) 222 °C				(d) 550 °C					
Cs1	0.3834(3)	0.7797(5)	0.6512(6)	5.50(20)	Cs1	0.3884(4)	0.7919(7)	0.6255(12)	8.0(4)
Cs2	0.1062(1)	0.6832(2)	0.9005(4)	2.98(7)	Cs2	0.1095(3)	0.6994(7)	0.8872(11)	6.4(2)
Ti1	0.3727(2)	0.4877(5)	0.0000	0.96(11)	Ti1	0.3722(2)	0.5000(9)	0.0000	1.8(2)
Ti2	0.2564(2)	0.2548(5)	0.7401(5)	0.97(10)	Ti2	0.2537(4)	0.2595(8)	0.7468(11)	1.8(1)
As1	0.5048(1)	0.3269(2)	0.7391(4)	0.89(7)	As1	0.5024(2)	0.3272(2)	0.7446(9)	1.6(1)
As2	0.3195(1)	0.9886(3)	0.9853(4)	0.92(6)	As2	0.3216(1)	0.9960(5)	0.9910(7)	1.7(1)
O1	0.4901(10)	0.464(3)	0.865(1)	1.9(6)	O1	0.490(2)	0.475(3)	0.868(2)	3.1(10)
O2	0.5165(10)	0.480(2)	0.618(1)	2.0(6)	O2	0.517(2)	0.467(5)	0.620(2)	3.6(12)
O3	0.4059(9)	0.179(2)	0.707(2)	1.8(5)	O3	0.398(2)	0.191(3)	0.720(3)	2.9(12)
O4	0.1091(9)	0.314(2)	0.751(1)	1.4(5)	O4	0.102(2)	0.320(3)	0.765(3)	2.7(10)
O5	0.3874(10)	0.785(2)	0.951(1)	1.7(5)	O5	0.388(2)	0.800(4)	0.953(2)	2.6(9)
O6	0.6113(10)	0.812(2)	0.524(2)	2.0(6)	O6	0.612(2)	0.802(3)	0.527(3)	4.2(14)
O7	0.2508(10)	0.032(2)	0.855(1)	2.0(6)	O7	0.250(2)	0.045(4)	0.864(2)	3.4(10)
O8	0.2638(9)	0.443(2)	0.597(1)	1.4(5)	O8	0.258(2)	0.451(4)	0.608(2)	2.6(9)
OT1	0.2217(10)	0.039(2)	0.602(1)	1.5(5)	OT1	0.217(2)	0.048(3)	0.609(2)	2.3(8)
OT2	0.2886(9)	0.432(2)	0.852(1)	1.5(5)	OT2	0.281(2)	0.437(4)	0.860(2)	2.2(8)

Refined occupancies of Cs1 at each temperature are 0.33(1), 0.31(2), 0.50(3), and 0.55(5) Cs and 0.67(1), 0.69(2), 0.50(3), and 0.45(5) K; those for Cs2 are 0.92(1), 0.91(2), 0.70(2), and 0.64(4) Cs and 0.08(1), 0.09(2), 0.30(2), and 0.34(4) K.

**Table 35B-2-002.** Cs<sub>0.6</sub>K<sub>0.4</sub>TiOAsO<sub>4</sub>, KTiOAsO<sub>4</sub>. Interatomic distances [Å] as a function of temperature [94Nor].

KTA

<i>T</i> [°C]					<i>T</i> [°C]				
	20	500	630	725		20	500	630	725
Ti(1)–O(1)	2.144(5)	2.124(15)	2.085(11)	2.18(3)	Ti(1)–O(6)	2.002(5)	2.004(15)	2.019(13)	2.02(3)
Ti(1)–O(2)	1.953(5)	2.000(16)	1.984(16)	1.97(2)	Ti(1)–O(T1)	1.724(5)	1.747(15)	1.759(13)	1.83(2)
Ti(1)–O(5)	2.039(4)	2.072(13)	2.065(10)	2.06(2)	Ti(1)–O(T2)	1.985(5)	1.967(14)	1.908(11)	1.85(2)
mean	1.974	1.986	1.970	1.986					
Ti(2)–O(3)	2.036(4)	2.029(13)	2.011(11)	2.04(2)	Ti(2)–O(8)	1.984(5)	1.969(17)	1.995(13)	1.94(3)
Ti(2)–O(4)	1.983(4)	2.006(12)	2.045(9)	2.01(2)	Ti(2)–O(T1)	2.106(5)	2.088(15)	2.053(14)	1.88(3)
Ti(2)–O(7)	1.972(5)	1.959(17)	1.967(12)	1.97(2)	Ti(2)–O(T2)	1.754(5)	1.768(17)	1.814(13)	1.96(3)
mean	1.972	1.970	1.981	1.97					
As(1)–O(1)	1.669(5)	1.671(16)	1.667(15)	1.69(4)	As(1)–O(3)	1.684(4)	1.690(13)	1.684(10)	1.69(2)
As(1)–O(2)	1.679(5)	1.653(19)	1.673(16)	1.67(2)	As(1)–O(4)	1.683(4)	1.690(12)	1.689(9)	1.70(2)
mean	1.679	1.676	1.678	1.69					
As(2)–O(5)	1.681(4)	1.675(12)	1.683(9)	1.68(2)	As(2)–O(7)	1.680(5)	1.700(16)	1.680(13)	1.67(2)
As(2)–O(6)	1.668(5)	1.677(15)	1.676(12)	1.66(2)	As(2)–O(8)	1.689(5)	1.686(15)	1.672(11)	1.73(3)
mean	1.680	1.684	1.678	1.68					
K(1)–O(1)	2.979(6)	3.20(3)	3.303(23)	3.45(5)	K(1)–O(7)	3.165(6)	3.302(22)	3.358(18)	3.42(4)
K(1)–O(2)	2.828(5)	2.731(22)	2.710(18)	2.74(2)	K(1)–O(8)	2.703(5)	2.752(18)	2.740(15)	2.73(3)
K(1)–O(3)	2.683(4)	2.716(15)	2.741(12)	2.73(3)	K(1)–O(T1)	2.890(5)	2.852(18)	2.846(15)	2.85(2)
K(1)–O(5)	2.883(5)	3.029(22)	3.130(17)	3.27(4)	K(1)–O(T2)	3.099(5)	3.277(21)	3.402(18)	3.56(4)
K(1)–O(6)	3.516(5)	3.384(19)	3.342(16)	3.32(3)					
mean	2.972	3.027	3.064	3.12					
K(2)–O(1)	2.662(5)	2.654(18)	2.692(17)	2.54(4)	K(2)–O(7)	2.907(5)	2.883(18)	2.885(14)	2.87(3)
K(2)–O(2)	2.969(6)	3.18(3)	3.280(23)	3.37(3)	K(2)–O(8)	3.127(6)	3.230(24)	3.224(20)	3.32(4)
K(2)–O(3)	3.149(6)	3.316(22)	3.319(20)	3.31(4)	K(2)–O(T1)	3.161(5)	3.258(19)	3.352(17)	3.49(3)
K(2)–O(4)	3.061(5)	2.969(16)	2.946(13)	2.99(3)	K(2)–O(T2)	2.854(5)	2.860(18)	2.867(15)	2.82(3)
K(2)–O(5)	2.836(5)	2.890(13)	2.881(12)	2.90(2)					
mean	2.970	3.027	3.050	3.07					

(continued)

Table 35B-2-002 (continued)

(Cs,K)TA

	<i>T</i> [°C]					<i>T</i> [°C]			
	20	222	400	550		20	222	400	550
Ti(1)–O(1)	2.123(8)	2.130(14)	2.119(14)	2.12(2)	Ti(1)–O(6)	2.031(8)	2.048(13)	2.053(12)	2.08(2)
Ti(1)–O(2)	1.954(8)	1.971(14)	1.962(16)	1.98(3)	Ti(1)–O(T1)	1.723(8)	1.720(13)	1.721(12)	1.70(2)
Ti(1)–O(5)	2.081(7)	2.074(13)	2.100(13)	2.11(3)	Ti(1)–O(T2)	1.979(8)	1.971(13)	1.963(12)	1.97(2)
mean	1.982	1.986	1.986	1.99					
Ti(2)–O(3)	2.078(7)	2.094(13)	2.055(12)	2.01(2)	Ti(2)–O(8)	1.998(8)	1.992(14)	1.981(13)	1.97(2)
Ti(2)–O(4)	2.016(7)	2.014(12)	2.057(12)	2.09(2)	Ti(2)–O(T1)	2.139(8)	2.123(14)	2.123(13)	2.12(2)
Ti(2)–O(7)	1.957(8)	1.946(15)	1.934(14)	1.92(3)	Ti(2)–O(T2)	1.747(8)	1.746(15)	1.744(13)	1.75(3)
mean	1.989	1.986	1.982	1.98					
As(1)–O(1)	1.666(8)	1.653(15)	1.650(15)	1.67(2)	As(1)–O(3)	1.689(7)	1.691(12)	1.685(13)	1.70(2)
As(1)–O(2)	1.693(8)	1.670(14)	1.675(17)	1.65(3)	As(1)–O(4)	1.686(7)	1.693(12)	1.693(12)	1.68(2)
mean	1.684	1.677	1.676	1.67					
As(2)–O(5)	1.678(7)	1.685(13)	1.676(12)	1.65(2)	As(2)–O(7)	1.693(8)	1.697(16)	1.699(13)	1.70(3)
As(2)–O(6)	1.680(8)	1.680(13)	1.692(13)	1.68(2)	As(2)–O(8)	1.678(8)	1.668(13)	1.674(12)	1.67(2)
mean	1.682	1.682	1.685	1.68					
Cs(1)–O(1)	3.297(9)	3.439(18)	3.572(18)	3.63(3)	Cs(1)–O(7)	3.242(8)	3.288(16)	3.484(13)	3.60(2)
Cs(1)–O(2)	2.749(9)	2.711(15)	2.752(14)	2.80(3)	Cs(1)–O(8)	2.809(8)	2.831(14)	2.879(15)	2.91(3)
Cs(1)–O(3)	2.761(8)	2.768(14)	2.845(14)	2.90(2)	Cs(1)–O(T1)	2.850(8)	2.828(14)	2.849(13)	2.89(2)
Cs(1)–O(5)	3.083(8)	3.216(17)	3.416(16)	3.49(3)	Cs(1)–O(T2)	3.319(9)	3.421(15)	3.642(15)	3.77(2)
Cs(1)–O(6)	3.437(9)	3.348(15)	3.220(15)	3.19(2)					
mean	3.061	3.094	3.184	3.24					
Cs(2)–O(1)	2.875(8)	2.859(15)	2.805(15)	2.74(2)	Cs(2)–O(7)	3.097(7)	3.077(13)	3.040(15)	3.02(3)
Cs(2)–O(2)	3.353(10)	3.484(17)	3.486(14)	3.52(3)	Cs(2)–O(8)	3.224(9)	3.247(16)	3.320(14)	3.42(3)
Cs(2)–O(3)	3.238(8)	3.293(16)	3.426(19)	3.56(3)	Cs(2)–O(T1)	3.253(8)	3.307(14)	3.391(13)	3.47(2)
Cs(2)–O(4)	2.984(8)	2.957(13)	2.911(13)	2.89(2)	Cs(2)–O(T2)	2.981(7)	3.013(13)	2.970(13)	2.93(2)
Cs(2)–O(5)	2.963(7)	2.985(13)	3.003(13)	3.06(2)					
mean	3.108	3.136	3.150	3.18					