

**Table 35A-20-001.** KTiOAsO<sub>4</sub>. Atomic position parameters [ $10^{-4}$ ] and temperature parameters  $B$  [ $\text{\AA}^2$ ] [86ElB]. For definition of  $B$ , see Eq. (e) in Introduction.

Atom	$x$	$y$	$z$	$B$
K <sub>1</sub>	3771(4)	3136(6)	7799(6)	1.89(7)
K <sub>2</sub>	1081(3)	689(6)	6996(7)	1.74(7)
Ti <sub>1</sub>	3750(1)	0	5066(7)	0.42(3)
Ti <sub>2</sub>	2464(3)	2484(6)	2697(5)	0.37(4)
As <sub>1</sub>	4980(2)	2575(6)	3288(2)	0.54(2)
As <sub>2</sub>	1809(1)	5104(5)	5071(4)	0.57(2)
O <sub>1</sub>	4868(12)	1447(14)	4935(32)	1.00(24)
O <sub>2</sub>	5065(12)	3916(14)	4711(34)	0.61(20)
O <sub>3</sub>	3921(10)	2781(16)	1792(22)	1.04(26)
O <sub>4</sub>	5973(10)	2388(16)	1756(24)	0.91(25)
OT <sub>1</sub>	2174(12)	3880(14)	539(32)	0.76(29)
OT <sub>2</sub>	2192(12)	6382(14)	−419(32)	0.96(30)
O <sub>5</sub>	1084(11)	5451(15)	3010(26)	0.75(24)
O <sub>6</sub>	1081(11)	4823(16)	7043(29)	0.82(24)
O <sub>7</sub>	2609(13)	6337(14)	5415(31)	0.84(26)
O <sub>8</sub>	2591(14)	3896(15)	4627(30)	0.79(27)

**Table 35A-20-002.** KTiOAsO<sub>4</sub>. Anisotropic temperature parameters [ $\cdot 10^{-4} \text{\AA}^2$ ] [86ElB]. For definition of  $\beta_{ij}$ , see Eq. (c) in Introduction.

Atom	$\beta_{11}$	$\beta_{22}$	$\beta_{33}$	$\beta_{12}$	$\beta_{13}$	$\beta_{23}$
K <sub>1</sub>	35(2)	46(3)	63(9)	12(3)	10(3)	13(5)
K <sub>2</sub>	18(2)	47(3)	106(10)	1(2)	3(5)	−3(5)
Ti <sub>1</sub>	6(1)	6(2)	31(5)	−4(2)	4(4)	4(3)
Ti <sub>2</sub>	4(1)	5(2)	42(6)	−2(2)	2(2)	1(4)
As <sub>1</sub>	7(1)	10(1)	43(2)	−1(1)	−1(2)	1(3)
As <sub>2</sub>	10(1)	8(1)	36(3)	1(1)	−1(3)	−2(1)
O <sub>1</sub>	15(7)	12(10)	114(45)	−7(7)	−6(2)	31(17)
O <sub>2</sub>	10(7)	12(9)	94(34)	4(7)	10(15)	−7(15)
O <sub>3</sub>	3(6)	27(12)	50(30)	−4(8)	−1(10)	−15(19)
O <sub>4</sub>	10(7)	14(11)	86(32)	6(8)	−2(12)	−18(19)
OT <sub>1</sub>	30(12)	3(12)	57(35)	−7(8)	1(17)	14(16)
OT <sub>2</sub>	3(9)	14(12)	85(40)	−10(7)	3(15)	−10(17)
O <sub>5</sub>	17(9)	12(10)	37(29)	3(8)	3(17)	−4(17)
O <sub>6</sub>	13(8)	20(12)	76(30)	−13(9)	21(17)	−1(19)
O <sub>7</sub>	6(9)	11(12)	103(37)	2(8)	−2(20)	−18(18)
O <sub>8</sub>	18(10)	10(12)	61(37)	9(8)	−22(21)	−19(16)

**Table 35A-20-003.** KTiOAsO<sub>4</sub>. Atomic coordinates and temperature parameters [94Nor]. *B*: isotropic temperature parameters [ $\text{\AA}^2$ ]. For definition of *B*, see Eq. (e) in Introduction.

$x$	$y$	$z$	$B$	$x$	$y$	$z$	$B$		
(a)				(b)					
K1	0.3766(1)	0.7791(2)	0.3129(2)	1.74(5)	K1	0.3811(6)	0.7819(10)	0.3321(11)	6.8(4)
K2	0.1079(1)	0.7000(2)	0.0684(2)	1.67(5)	K2	0.1083(5)	0.7019(10)	0.0856(10)	5.9(4)
Ti1	0.3748(1)	0.5065(2)	0.00000	0.37(3)	Ti1	0.8736(2)	0.9963(4)	0.00000	1.2(1)
Ti2	0.2467(1)	0.2714(1)	0.2493(2)	0.36(3)	Ti2	0.2495(2)	0.2664(4)	0.2501(5)	1.2(1)
As1	0.49790(4)	0.3290(1)	0.2591(2)	0.33(2)	As1	0.4995(1)	0.3277(2)	0.2577(5)	1.12(4)
As2	0.18113(3)	0.5071(1)	0.5118(1)	0.36(2)	As2	0.1801(1)	0.5029(2)	0.5107(4)	1.19(4)
O1	0.9878(4)	0.0026(8)	0.1437(5)	0.77(14)	O1	0.9889(13)	0.014(3)	0.1375(17)	2.5(6)
O2	0.5067(4)	0.4612(8)	0.3920(5)	0.89(15)	O2	0.5081(11)	0.467(4)	0.3848(19)	2.9(7)
O3	0.3937(3)	0.1819(6)	0.2765(5)	0.68(15)	O3	0.3956(10)	0.182(2)	0.2773(18)	2.3(6)
O4	0.0984(3)	0.3268(7)	0.2383(5)	0.68(14)	O4	0.1008(9)	0.324(2)	0.2343(15)	1.7(5)
O5	0.3924(3)	0.8054(7)	0.0466(4)	0.66(13)	O5	0.3910(9)	0.804(2)	0.0508(17)	2.3(6)
O6	0.6053(3)	0.7945(7)	0.4828(5)	0.84(15)	O6	0.6082(13)	0.795(2)	0.4781(16)	2.7(6)
O7	0.2391(4)	0.0414(8)	0.1319(5)	0.74(15)	O7	0.2407(10)	0.040(3)	0.1334(16)	2.4(6)
O8	0.2592(4)	0.4651(8)	0.3898(5)	0.77(15)	O8	0.2583(13)	0.459(3)	0.3895(17)	2.8(6)
OT1	0.2163(4)	0.0545(8)	0.3885(5)	0.77(14)	OT1	0.2195(12)	0.053(3)	0.3885(15)	1.9(5)
OT2	0.2789(4)	0.4574(8)	0.1393(5)	0.66(14)	OT2	0.2805(12)	0.454(3)	0.1396(15)	2.1(5)
(c)				(d)					
K1	0.3821(6)	0.7831(8)	0.3366(10)	9.4(4)	K1	0.3816(11)	0.785(2)	0.347(2)	12.4(12)
K2	0.1086(5)	0.7024(10)	0.0881(9)	8.2(4)	K2	0.1077(8)	0.706(3)	0.094(2)	11.4(12)
Ti1	0.8731(1)	0.9971(4)	0.0000	1.63(6)	Ti1	0.3725(2)	0.501(1)	0.0000	2.1(2)
Ti2	0.2506(2)	0.2626(3)	0.2508(4)	1.70(5)	Ti2	0.2505(5)	0.251(1)	0.2526(11)	2.3(1)
As1	0.4998(1)	0.3278(1)	0.2559(4)	1.48(3)	As1	0.5006(2)	0.3278(2)	0.2540(9)	1.86(5)
As2	0.1801(1)	0.5014(2)	0.5083(3)	1.55(3)	As2	0.1798(1)	0.4987(5)	0.5034(9)	1.9(1)
O1	0.9883(10)	0.023(3)	0.1317(14)	3.4(6)	O1	0.9892(16)	0.017(6)	0.129(4)	6.0(13)
O2	0.5124(12)	0.476(3)	0.3813(16)	3.6(6)	O2	0.5172(12)	0.477(3)	0.378(2)	2.4(6)
O3	0.3959(8)	0.186(2)	0.2792(15)	3.2(5)	O3	0.3986(13)	0.183(4)	0.286(2)	2.7(7)
O4	0.0998(6)	0.327(1)	0.2350(11)	2.0(4)	O4	0.1033(15)	0.324(3)	0.241(2)	2.6(7)
O5	0.3934(8)	0.803(1)	0.0457(12)	2.5(4)	O5	0.3927(11)	0.801(3)	0.042(2)	2.5(7)
O6	0.6076(10)	0.797(2)	0.4771(14)	3.6(5)	O6	0.6126(23)	0.798(4)	0.468(3)	6.6(15)
O7	0.2420(11)	0.040(2)	0.1296(12)	2.8(4)	O7	0.2445(14)	0.037(4)	0.125(2)	3.2(8)
O8	0.2604(10)	0.460(2)	0.3907(13)	3.3(5)	O8	0.2617(16)	0.456(4)	0.380(3)	4.0(10)
OT1	0.2168(10)	0.048(2)	0.3825(14)	2.7(5)	OT1	0.2152(17)	0.055(3)	0.372(3)	2.7(7)
OT2	0.2804(9)	0.448(2)	0.1319(13)	2.4(4)	OT2	0.2764(16)	0.452(4)	0.122(3)	3.0(8)

**Table 35A-20-004.** KTiOAsO<sub>4</sub>. Bond distances and angles in AsO<sub>4</sub><sup>3-</sup> tetrahedra [86ElB].

As <sub>1</sub> –O <sub>4</sub> [Å]	As <sub>2</sub> –O <sub>4</sub> [Å]
As <sub>1</sub> –O <sub>1</sub> = 1.630(19)	As <sub>2</sub> –O <sub>5</sub> = 1.694(16)
As <sub>1</sub> –O <sub>2</sub> = 1.720(18)	As <sub>2</sub> –O <sub>6</sub> = 1.635(18)
As <sub>1</sub> –O <sub>3</sub> = 1.714(14)	As <sub>2</sub> –O <sub>7</sub> = 1.704(16)
As <sub>1</sub> –O <sub>4</sub> = 1.656(14)	As <sub>2</sub> –O <sub>8</sub> = 1.679(18)
O–As <sub>1</sub> –O [°]	O–As <sub>2</sub> –O [°]
O <sub>1</sub> –As <sub>1</sub> –O <sub>2</sub> = 105.6(9)	O <sub>5</sub> –As <sub>2</sub> –O <sub>6</sub> = 110.2(8)
O <sub>1</sub> –As <sub>1</sub> –O <sub>3</sub> = 113.7(8)	O <sub>5</sub> –As <sub>2</sub> –O <sub>7</sub> = 106.2(9)
O <sub>1</sub> –As <sub>1</sub> –O <sub>4</sub> = 112.5(9)	O <sub>5</sub> –As <sub>2</sub> –O <sub>8</sub> = 112.0(9)
O <sub>2</sub> –As <sub>1</sub> –O <sub>3</sub> = 104.8(8)	O <sub>6</sub> –As <sub>2</sub> –O <sub>7</sub> = 113.4(9)
O <sub>2</sub> –As <sub>1</sub> –O <sub>4</sub> = 112.3(8)	O <sub>6</sub> –As <sub>2</sub> –O <sub>8</sub> = 110.5(9)
O <sub>3</sub> –As <sub>1</sub> –O <sub>5</sub> = 107.7(7)	O <sub>7</sub> –As <sub>2</sub> –O <sub>8</sub> = 104.4(8)

**Table 35A-20-005.** KTiOAsO<sub>4</sub>. Bond distances in TiO<sub>6</sub> octahedra [86ElB].

Ti <sub>1</sub> –O [Å]	Ti <sub>2</sub> –O [Å]
Ti <sub>1</sub> –O <sub>1</sub> = 2.138(15)	Ti <sub>2</sub> –O <sub>3</sub> = 2.025(14)
Ti <sub>1</sub> –O <sub>2</sub> = 2.947(16)	Ti <sub>2</sub> –O <sub>4</sub> = 1.989(14)
Ti <sub>1</sub> –OT <sub>1</sub> = 1.735(16)	Ti <sub>2</sub> –OT <sub>1</sub> = 2.097(19)
Ti <sub>1</sub> –OT <sub>2</sub> = 1.957(16)	Ti <sub>2</sub> –OT <sub>2</sub> = 1.770(19)
Ti <sub>1</sub> –O <sub>5</sub> = 2.002(18)	Ti <sub>2</sub> –O <sub>7</sub> = 1.941(19)
Ti <sub>1</sub> –O <sub>6</sub> = 2.004(19)	Ti <sub>2</sub> –O <sub>8</sub> = 1.983(18)

**Table 35A-20-006.** KTiOAsO<sub>4</sub>, K<sub>0.4</sub>Cs<sub>0.6</sub>TiOAsO<sub>4</sub>. Interatomic distances [Å] as a function of temperature [94Nor].

(a)

KTiOAsO <sub>4</sub>									
	<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					

Table 35A-20-006 (continued)  
(b)

K <sub>0.4</sub> Cs <sub>0.6</sub> TiOAsO <sub>4</sub>									
	<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(6)	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					

**Table 35A-20-007.** KTiOAsO<sub>4</sub>. Atomic coordinates [94May].

	$x$	$y$	$z$
K(1)	0.37725(9)	0.7802(1)	0.6856(1)
K(2)	0.10748(7)	0.6977(2)	0.9288(1)
Ti(1)	0.37445(4)	0.50584(8)	−0.00233(8)
Ti(2)	0.24717(4)	0.26783(7)	0.74776(8)
As(1)	0.49807(3)	0.33035(4)	0.74007(8)
As(2)	0.18139(2)	0.50645(5)	0.48803(7)
O(1)	0.4871(2)	0.4948(4)	0.8562(3)
O(2)	0.5066(2)	0.4659(5)	0.6072(2)
O(3)	0.3939(2)	0.1822(4)	0.7214(3)
O(4)	0.5988(2)	0.1738(4)	0.7599(3)
O(5)	0.2206(2)	0.9569(5)	0.3601(2)
O(6)	0.2177(2)	0.0555(5)	0.6101(2)
O(7)	0.1081(2)	0.3057(4)	0.4517(2)
O(8)	0.1057(2)	0.7065(4)	0.5160(3)
O(9)	0.2620(2)	0.5414(5)	0.3664(2)
O(10)	0.2596(2)	0.4648(5)	0.6088(2)

**Table 35A-20-008.** KTiOAsO<sub>4</sub>. Anisotropic temperature parameters [ $\text{\AA}^2$ ] [94May]. For definition of  $U_{ij}$ , see Eq. (d) in Introduction.

	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
K(1)	0.0404(6)	0.0160(4)	0.0357(5)	−0.0033(4)	−0.0105(4)	0.0037(4)
K(2)	0.0175(4)	0.0253(4)	0.0404(5)	0.0008(4)	−0.0002(4)	0.0052(3)
Ti(1)	0.0045(2)	0.0047(2)	0.0060(2)	−0.0006(2)	0.0002(2)	−0.0003(2)
Ti(2)	0.0035(2)	0.0064(2)	0.0056(2)	0.0019(2)	−0.0009(1)	−0.0007(1)
As(1)	0.0040(1)	0.0063(1)	0.0069(1)	−0.0004(2)	0.0070(9)	−0.0002(1)
As(2)	0.0069(1)	0.0047(1)	0.0068(1)	0.0007(1)	−0.0005(1)	−0.0005(1)
O(1)	0.013(1)	0.014(2)	0.012(1)	−0.0070(9)	0.003(1)	−0.0039(9)
O(2)	0.007(1)	0.015(1)	0.014(1)	0.007(1)	0.0021(9)	0.0031(9)
O(3)	0.0046(9)	0.010(1)	0.015(2)	−0.0006(9)	−0.0023(9)	−0.0003(7)
O(4)	0.0044(9)	0.009(1)	0.015(2)	0.0032(9)	−0.0009(9)	−0.0006(7)
O(5)	0.005(1)	0.012(1)	0.011(1)	0.001(1)	0.0027(8)	0.001(1)
O(6)	0.015(1)	0.009(1)	0.011(1)	−0.004(1)	−0.0049(9)	0.001(1)
O(7)	0.010(1)	0.0036(9)	0.017(2)	−0.0018(9)	−0.0036(9)	−0.0035(8)
O(8)	0.014(1)	0.008(1)	0.017(2)	0.002(1)	0.005(1)	0.0021(9)
O(9)	0.010(2)	0.013(1)	0.009(1)	0.0050(9)	0.0049(9)	0.004(1)
O(10)	0.013(2)	0.010(1)	0.012(1)	0.0050(9)	−0.007(1)	−0.004(1)

**Table 35A-20-009.** KTiOAsO<sub>4</sub>. Bond lengths [Å] around Ti and As [94May].

The symmetry operators given refer to the O atoms.

Around Ti(1)		Around Ti(2)	
O(1 <sup>i</sup> )	2.126(3)	O(3)	2.028(2)
O(2 <sup>ii</sup> )	1.967(3)	O(4 <sup>v</sup> )	1.990(2)
O(5 <sup>iii</sup> )	1.966(3)	O(5 <sup>vi</sup> )	1.787(3)
O(6 <sup>iv</sup> )	1.744(3)	O(6)	2.075(3)
O(7 <sup>iv</sup> )	2.047(3)	O(9 <sup>vi</sup> )	1.967(3)
O(8 <sup>iii</sup> )	1.997(3)	O(10)	1.988(3)
Around As(1)			
O(1)	1.661(3)	O(7)	1.681(2)
O(2)	1.692(3)	O(8)	1.676(3)
O(3)	1.691(2)	O(9)	1.701(3)
O(4)	1.690(2)	O(10)	1.681(3)

Symmetry codes: (i)  $x, y, z - 1$ ; (ii)  $-x + 1, -y + 1, z - \frac{1}{2}$ ;

(iii)  $-x + \frac{1}{2}, y - \frac{1}{2}, z - \frac{1}{2}$ ; (iv)  $-x + \frac{1}{2}, y + \frac{1}{2}, z - \frac{1}{2}$ ,

(v)  $x - \frac{1}{2}, -y + \frac{1}{2}, z$ ; (vi)  $-x + \frac{1}{2}, y - \frac{1}{2}, z + \frac{1}{2}$ .

**Table 35A-20-010.** KTiOAsO<sub>4</sub>. Coefficients for the thermal expansion in reference to 25 °C [94Zho].  $\Delta l/l_{25} = a + bT + cT^2 + dT^3$ ;  $T$  is the temperature [K]. Effective temperature range: 103 to 1073 K.

Axis	$a$	$b$ [K <sup>-1</sup> ]	$c$ [K <sup>-2</sup> ]	$d$ [K <sup>-3</sup> ]
a	$-1.5420 \cdot 10^{-3}$	$2.20972 \cdot 10^{-6}$	$1.12511 \cdot 10^{-8}$	$-4.6042 \cdot 10^{-12}$
b	$-2.5298 \cdot 10^{-3}$	$5.98544 \cdot 10^{-6}$	$9.66804 \cdot 10^{-9}$	$-3.6037 \cdot 10^{-12}$
c	$-4.0622 \cdot 10^{-4}$	$3.51577 \cdot 10^{-6}$	$-5.8902 \cdot 10^{-9}$	$-2.1710 \cdot 10^{-12}$

**Table 35A-20-011.** KTiOAsO<sub>4</sub>. Coefficients for the thermal expansion in reference to 258 °C [94Zho].  $\Delta l/l_{25} = a + bT + cT^2 + dT^3$ ;  $T$  is the temperature [K]. Effective temperature range: 1173 to 1223 K.

Axis	$a$	$b$ [K <sup>-1</sup> ]	$c$ [K <sup>-2</sup> ]	$d$ [K <sup>-3</sup> ]
a	$6.78380 \cdot 10^{-1}$	$-1.7512 \cdot 10^{-3}$	$1.51895 \cdot 10^{-6}$	$-4.3709 \cdot 10^{-10}$
b	$-1.3986 \cdot 10^{-0}$	$3.4169 \cdot 10^{-3}$	$-2.7609 \cdot 10^{-6}$	$7.44309 \cdot 10^{-10}$
c	$1.95081 \cdot 10^{-1}$	$-5.4428 \cdot 10^{-4}$	$4.87860 \cdot 10^{-7}$	$-1.4574 \cdot 10^{-10}$

**Table 35A-20-012.** KTiOAsO<sub>4</sub>. Raman modes [91Wat]. Roman numerals simply classify the frequency ranges. w: weak; m: medium; s: strong; v: very.  $\nu$ : frequency of Raman modes [cm<sup>-1</sup>].

KTA	A <sub>1</sub> x(zz)y			A <sub>1</sub> z(xx)y			A <sub>1</sub> x(yy)z			B <sub>2</sub> x(zy)z			B <sub>1</sub> x(zz)z			A <sub>2</sub> x(yx)z		
	$\nu$	HW	Amp.	$\nu$	HW	Amp.	$\nu$	HW	Amp.	$\nu$	HW	Amp.	$\nu$	HW	Amp.	$\nu$	HW	Amp.
I	41.0	1.2	vw	41.2	1.3	ms							41.4	1.3	vw			
	64.8	1.4	–	64.8	1.3	vw				62.6	1.4	vw	54.0		vw	54.0	1.1	vvs
	72.8	2.8	vww				70.6	1.9	w	71.8	1.4	vw				71.4	1.8	s
				76.0	2.3	vs	76.0	2.2	m				75.8	2.4	m	75.6	2.9	m
				82.2	1.4	ms	81.6	1.4	vw									
				89.0	1.3	m				81.0	1.5	ms						
	92.6	1.0	mw	92.8	1.2	vs	93.0	1.4	w	90.4	1.8	w	87.4	1.8	vvs			
	99.6	1.2	mw	100.0	1.4	s	100.2	1.2	mw				94.4	1.2	ms			
	104.6	2.7	–	105.4	2.5	w	104.6	2.0	w				100.0	0.7	w	102.4	1.4	s
										108.6	2.7	mw	103.8	2.3	w			
II				113.4	2.0	s	113.6	2.1	ms				112.0	1.9	w	111.6	1.4	vvs
	133.0	1.9	mw	133.0	2.4	mw	133.0	2.0	s				119.8	1.8	s	116.6	1.9	vs
				136.6	1.1	vw	138.6	2.0	mw	136.0	1.4	ms				130.6	2.1	m
				145.4	1.8	mw	145.8	2.5	mw				135.6	0.9	vw	146.6	3.2	ms
	154.6	2.9	vw	154.6	4.5	w				151.4	3.0	mw	150.6	2.4	vs			
				169.0	1.8	w				158.4	2.4	m						
	176.0	2.8	m	176.8	2.5	s	176.8	2.9	ms	164.8	3.1	s	164.4	3.2	vw			
										185.0	3.6	ms	176.0	2.5	vs	176.6	2.4	ms
	189.2	2.4	s	189.4	2.7	ms	189.6	2.4	vs	188.4	2.5	s	188.4	3.4	m	189.2	3.0	m
				207.0	3.1	mw	205.0	3.4	mw	205.0	3.0	vvs	205.6	3.1	m	208.0	6.1	w
	211.8	3.0	w				212.6	2.4	ms	219.8	3.6	m	213.0	2.4	mw			
				219.8	3.1	m	219.8	3.6	m	220.8	3.5	mw						
				224.6	2.7	mw	224.4	2.1	ms				223.2	3.0	m	223.6	2.7	vs

(continued)



Table 35A-20-012 (continued)

KTA	A <sub>1</sub> x(zz)y			A <sub>1</sub> z(xx)y			A <sub>1</sub> x(yy)z			B <sub>2</sub> x(zy)z			B <sub>1</sub> x(zz)z			A <sub>2</sub> x(yx)z		
	v	HW	Amp.	v	HW	Amp.	v	HW	Amp.	v	HW	Amp.	v	HW	Amp.	v	HW	Amp.
III	234.0	2.8	vvs				239.0	3.1	ms	240.4	3.0	ms	240.6	3.9	ms	234.8	2.6	vs
	247.4	1.9	m	238.6	4.6	w	250.2	2.4	m	250.0	2.6	vs	250.2	2.7	ms	247.8	2.3	vvs
				248.0	2.2	mw	255.8	2.6	mw									
				255.8	2.6	mw	261.4	2.4	mw	262.0	2.4	m	260.4	2.4	ms			
IV	272.4	2.5	s	270.0	3.7	m	269.2	2.8	ms	270.2	2.5	s	269.4	3.1	vvs	270.4	3.6	vs
	284.4	2.5	m	279.8	2.7	m	280.0	3.1	m	290.6	5.3	w	295.6	2.9	m	299.4	3.8	s
				297.2	3.2	m	304.6	6.9	m	307.2	5.5	ms	311.4	6.6	m			
	308.8	2.8	vvw	308.4	2.5	w	310.2	2.6	m	310.6	3.8	vs	315.8	2.4	m	313.6	2.9	vs
V	329.4	4.0	mw				329.4	5.1	s	325.2	4.2	s	326.0	4.9	w	320.6	3.4	vs
	342.6	4.8	ms				343.0	4.8	vs							342.0	5.7	m
				342.8	4.7	vs				347.2	3.5	m						
	360.2	3.5	vvw				360.0	2.9	w	362.8	2.8	mw	359.2	5.0	m	359.6	4.1	s
VI	372.2	3.5	m	370.8	3.5	vs				369.0	6.0	vvw	372.0	4.6	ms	387.2	5.9	m
	384.2	4.6	–				384.2	4.2	ms									
													395.6	3.4	mw			
				419.4	3.3	s				410.0	4.8	w	407.2	5.0	w	413.0	2.4	vvw
	437.2	5.1	vvw	433.0	7.8	m	436.4	3.8	vvw	420.8	2.9	vvw	435.6	4.0	ms	434.6	4.2	w
				451.6	2.4	vvw	444.4	3.3	mw	436.6	3.9	mw	447.6	4.5	mw	443.6	3.2	m
	460.8	4.7	–	465.2	5.9	mw	462.8	4.6	m	443.0	4.7	vvw	463.8	5.3	vvw	458.8	4.0	mw
				478.4	3.5	mw	481.6	4.4	mw	463.8	5.3	vvw	481.0	7.8	m			

(continued)

Table 35A-20-012 (continued)

KTA	A <sub>1</sub> x(zz)y			A <sub>1</sub> z(xx)y			A <sub>1</sub> x(yy)z			B <sub>2</sub> x(zy)z			B <sub>1</sub> x(zz)z			A <sub>2</sub> x(yx)z		
	v	HW	Amp.	v	HW	Amp.	v	HW	Amp.	v	HW	Amp.	v	HW	Amp.	v	HW	Amp.
VIIa	491.8	3.3	vw	491.2	3.3	vvs	491.2	3.6	s	490.2	4.8	–				490.4	3.2	w
	505.4	6.5	mw	509.8	9.5	s	506.2	5.5	m							509.6	5.6	w
	514.4	3.2	–	513.4	3.7	ms	513.2	4.5	m	515.4	6.4	m	513.2	3.3	vvw			
VIIb							531.6	10.4	m	535.0	6.2	m	531.8	9.6	m	533.4	9.9	vw
																552.8	5.2	w
	669.8	10.0	vs	673.0	10.3	vs	676.2	13.2	m	674.0	10.6	vvs	673.8	10.9	m	674.8	6.4	w
VIII				722.4	8.6	vvs	703.6	9.5	vvs				700.4	13.9	w	704.2	9.4	m
							747.6	7.0	w	747.0		–	747.4	6.6	vvs	746.8	5.5	vs
	772.8	3.7	vvw	777.0	5.1	m	776.8	5.9	mw	773.2	4.1	mw	774.8	9.3	w	781.8	6.7	ms
IX				798.6	5.3	m				794.6	4.9	mw	796.4	5.1	w			
							803.4	6.6	ms									
	8060.0	6.6	w				810.2	4.4	ms	806.2	8.3	vvw	810.2	4.7	s	809.2	5.3	vvs
				816.8	4.4	s	818.4	5.1	m									
				829.2	3.9	m	827.8	4.5	m	827.4	5.8	vw				828.8	6.2	mw
										836.8	4.6	mw	837.6	8.8	w			
	847.6	4.3	vvw	844.8	4.6	s	843.4	6.1	w							846.6	3.6	m
	874.6	4.2	–	873.6	4.2	ms	873.2	4.2	m	872.8	3.4	vvw	874.8	4.4	s	874.4	6.8	mw
	891.6	5.5	vvw	890.0	5.1	ms	889.6	6.0	w	882.0	5.5	–	884.2	9.6	w	885.8	4.0	ms
				907.4	3.4	w	907.6	4.9	m	907.4	5.4	–	906.8	5.1	w			
				916.8	5.5	m												
	939.8	–	–				939.4	6.0	mw				930.4	7.0	mw	928.4	5.7	mw
										950.2	7.5	–	946.4	5.5	m	937.0	4.8	mw