Table 35A-22-001. $CsTiOAsO_4$. Atomic positions and isotropic equivalent temperature parameters [89Pro]. For definition of *B*, see Eq. (e) in Introduction. O(T1), O(T2): oxygens of Ti(1) side and Ti(2) side, respectively.

	x	*y*	*z*	*B* [Å]
Ti(1)	0.37236(6)	0	0.5032(1)	0.482(9)
Ti(2)	0.25168(7)	0.25165(9)	0.2655(1)	0.449(9)
As(1)	0.50117(4)	0.25561(6)	0.32609(6)	0.406(5)
As(2)	0.17764(3)	0.51011(6)	0.50102(8)	0.449(5)
Cs(1)	0.38665(3)	0.35427(6)	0.78585(5)	1.851(7)
Cs(2)	0.11062(3)	0.09679(5)	0.69831(5)	1.420(5)
O(1)	0.4861(3)	0.1359(4)	0.4754(7)	1.05(6)
O(2)	0.5154(3)	0.3884(4)	0.4605(6)	1.00(6)
O(3)	0.3977(3)	0.2819(4)	0.1911(6)	0.85(5)
O(4)	0.6023(3)	0.2359(4)	0.1841(6)	0.93(6)
O(T1)	0.2158(3)	0.6411(4)	–0.0580(6)	0.75(5)
O(T2)	0.2176(3)	0.3923(4)	0.0577(6)	0.82(5)
O(5)	0.1106(3)	0.5481(4)	0.3012(6)	0.95(5)
O(6)	0.1108(3)	0.4734(4)	0.7008(6)	0.91(5)
O(7)	0.2543(3)	0.6356(4)	0.5476(6)	0.96(6)
O(8)	0.2560(3)	0.3940(4)	0.4488(6)	0.88(5)

Table 35A-22-002. $CsTiOAsO_4$, $KTiOAsO_4$, $KTiOPO_4$. Comparison between the various values of the two TiO_6 octahedra [89Pro]. G: center of the Ti-oxygen octahedron. O(T1), O(T2): oxygens of Ti(1) side and Ti(2) side, respectively.

	$CsTiOAsO_4$	$KTiOAsO_4$	$KTiOPO_4$
Length [Å] Ti(1)–O(T2)	1.714	1.735	1.716
Distance [Å] Ti(1)–G	0.23	0.17	0.23
Volume [$Å^3$] $Ti(1)O_6$	10.37	9.90	10.13
Angle [°] Ti(2)–O(T2), b	132.20	133.92	132.48
Length [Å] Ti(2)–O(T1)	1.748	1.770	1.735
Distance [Å] Ti(2)–G	0.16	0.17	0.18
Volume [$Å^3$] $Ti(2)O_6$	10.32	10.05	10.10
Angle [°] Ti(2)–O(T1), b	132.53	132.00	130.92
Angle [°] between the planes containing Ti(1)–O(T2) and Ti(2)–O(T1)	92.78	92.28	94.19

Table 35A-22-003. $CsTiOAsO_4$. Bond lengths [Å] angles [°] in the octahedra $Ti(1)O_6$ and $Ti(2)O_6$ and in the tetrahedra $As(1)O_4$ and $As(2)O_4$ and the polyhedra of Cs(1) and Cs(2) [89Pro].

Ti(1)	O(1)	O(2)	O(5)	O(6)	O(T1)	O(T2)
O(1)	2.121(5)	2.729(6)	2.753(6)	2.875(6)	2.733(6)	–
O(2)	82.5(2)	1.943(5)	2.791(6)	2.808(6)	–	2.730(6)
O(5)	80.9(2)	86.6(2)	2.121(4)	–	3.012(6)	2.765(6)
O(6)	85.7(2)	87.7(2)	166.7(2)	2.106(4)	2.820(6)	2.972(6)
O(T1)	83.8(2)	165.8(2)	94.9(2)	87.6(2)	1.966(4)	2.776(6)
O(T2)	172.5(2)	96.4(2)	91.6(2)	101.6(2)	97.7(2)	1.714(4)

Ti(2)	O(3)	O(4)	O(7)	O(8)	O(T1)	O(T2)
O(3)	2.059(4)	–	2.760(6)	2.865(6)	2.751(6)	2.850(6)
O(4)	173.5(2)	2.050(4)	2.877(6)	2.824(6)	2.791(6)	2.888(6)
O(7)	87.1(2)	92.1(2)	1.945(5)	–	2.756(6)	2.771(6)
O(8)	90.5(2)	89.1(2)	169.3(2)	1.974(4)	2.730(6)	2.732(6)
O(T1)	92.2(2)	94.3(2)	96.4(2)	94.2(2)	1.748(4)	–
O(T2)	85.9(2)	87.6(2)	85.8(2)	83.6(2)	177.1(2)	2.122(5)

As(1)	O(1)	O(2)	O(3)	O(4)
O(1)	1.652(5)	2.682(6)	2.768(6)	2.756(8)
O(2)	108.9(2)	1.703(5)	2.689(6)	2.761(1)
O(3)	111.4(2)	104.4(2)	1.698(4)	2.805(6)
O(4)	111.2(2)	108.9(2)	111.7(2)	1.690(4)

As(2)	O(5)	O(6)	O(7)	O(8)
O(5)	1.691(4)	2.855(6)	2.735(6)	2.753(6)
O(6)	115.4(2)	1.687(4)	2.801(6)	2.747(6)
O(7)	106.5(2)	110.5(2)	1.722(5)	2.669(6)
O(8)	110.0(2)	109.9(2)	103.8(2)	1.669(4)

Cs(1)			Cs(2)		
	O(1)	3.433(5)		O(1)	2.830(5)
	O(2)	2.852(5)		O(2)	3.330(5)
	O(3)	2.890(5)		O(3)	3.368(5)
	O(5)	3.274(5)		O(4)	2.966(4)
	O(6)	3.281(4)		O(5)	3.028(5)
	O(7)	3.507(5)		O(7)	3.039(5)
	O(8)	2.938(4)		O(8)	3.300(4)
	O(T1)	3.559(4)		O(T1)	2.966(4)
	O(T2)	2.974(4)		O(T2)	3.328(4)