Table 35B-1-001. $KM_{0.5}M'_{0.5}OPO_4$ and $K_{0.5}M_{0.5}M'_{0.5}OPO_4$. Composition, color, lattice parameters [Å], reducing power [94Gop].

Composition	Color	Reducing power		Lattice parameters [Å]		
		Found	Expected [a])	*a*	*b*	*c*
$KNb_{0.5}Ti_{0.5}OPO_4$	Dark blue	0.48	0.50	12.976(5)	6.488(4)	10.773(7)
$KNb_{0.5}V_{0.5}OPO_4$	Brown	1.02	1.0	12.949(6)	6.431(8)	10.686(4)
$KNb_{0.5}Cr_{0.5}OPO_4$	Green	–	–	12.894(7)	6.435(6)	10.629(6)
$KNb_{0.5}Fe_{0.5}OPO_4$	Orange	–	–	12.956(9)	6.467(5)	10.698(8)
$KTa_{0.5}Ti_{0.5}OPO_4$	Black	0.47	0.50	12.981(8)	6.484(7)	10.763(8)
$KTa_{0.5}V_{0.5}OPO_4$	Grey	0.98	1.00	12.985(4)	6.442(3)	10.696(4)
$KTa_{0.5}Cr_{0.5}OPO_4$	Green	–	–	12.914(5)	6.433(3)	10.670(6)
$KTa_{0.5}Fe_{0.5}OPO_4$	Orange	–	–	13.045(7)	6.450(8)	10.662(6)
$K_{0.5}Nb_{0.5}Ti_{0.5}OPO_4$	White	–	–	12.879(9)	6.402(7)	10.659(4)
$K_{0.5}Nb_{0.5}V_{0.5}OPO_4$	Yellowish green	0.52	0.50	12.801(6)	6.357(4)	10.569(5)
$K_{0.5}Ta_{0.5}Ti_{0.5}OPO_4$	White	–	–	12.852(9)	6.409(8)	10.663(6)
$K_{0.5}Ta_{0.5}V_{0.5}OPO_4$	Yellow	0.54	0.50	12.819(7)	6.367(4)	10.615(5)

[a]) Corresponds to the number of electrons per formula unit required for the oxidation of titanium/vanadium.

Table 35B-1-002. $K_{1-x}Ti_{1-y}V_yOPO_4$. Composition, color, reducing power, lattice parameters and SHG intensity [94Gop].

Composition	Color	Reducing power		Lattice parameters [Å]			SHG intensity [b])
		Found	Expected [a])	*a*	*b*	*c*	
$KTi_{0.85}V_{0.15}OPO_4$	Yellow	0.15	0.15	12.808(5)	6.400(6)	10.578(6)	0.10
$K_{0.85}Ti_{0.85}V_{0.15}OPO_4$	Yellow	0.01	0.00	12.800(6)	6.364(3)	10.572(8)	0.36
$KTi_{0.75}V_{0.25}OPO_4$	Brown	0.26	0.25	12.812(6)	6.401(6)	10.569(8)	0.05
$K_{0.75}Ti_{0.75}V_{0.25}OPO_4$	Yellowish green	0.02	0.00	12.723(8)	6.340(5)	10.561(8)	0.24
$KTi_{0.50}V_{0.50}OPO_4$	Brown	0.48	0.50	12.799(7)	6.390(6)	10.560(4)	–
$K_{0.67}Ti_{0.50}V_{0.50}OPO_4$	Green	0.17	0.00	12.716(4)	6.363(3)	10.529(5)	0.20

[a]) Expected for complete oxidation of vanadium.
[b]) Normalized with respect to that of $KTiOPO_4$ (hydrothermally synthesized) which is taken as unity.

Table 35B-1-003. $K_{1-x}Na_xTiOPO_4$ (ceramics). Lattice constants, T_{melt}, Θ_f [90Vor]. T_{melt}: melting temperature, Θ_f: ferroelectric transition temperature.

x	a [nm]	b [nm]	c [nm]	T_{melt} [°C]	Θ_f [°C]
0	1.286	0.645	1.063	1135	931
0.1	1.283	0.644	1.060	1120	936
0.2	1.284	0.642	1.062	1110	–
0.3	1.280	0.638	1.061	1090	946
0.4	1.282	0.639	1.063	1068	–
0.5	1.282	0.637	1.064	1048	953
0.6	1.278	0.635	1.063	1028	–
0.7	1.277	0.628	1.060	985	984
0.8	1.269	0.626	1.050	980	–
0.9	1.266	0.629	1.051	975	–
1	–	–	–	964	–

Table 35B-1-004. $K_{1-x}Tl_xTiOPO_4$ (ceramics). Lattice constants, Θ_f [90Vor].

x	a [nm]	b [nm]	c [nm]	Θ_f [°C]
0	1.285	0.642	1.063	919
0.1	1.286	0.643	1.062	880
0.2	1.287	0.643	1.061	851
0.3	1.289	0.644	1.062	825
0.4	1.290	0.645	1.060	791
0.5	1.292	0.646	1.059	718
0.6	1.294	0.647	1.059	706
0.7	1.295	0.647	1.059	664
0.8	1.295	0.648	1.060	627
0.9	1.297	0.649	1.060	604
1	1.297	0.649	1.058	565

Table 35B-1-005. $K_{1-x}Na_xTiOPO_4$. Variation of lattice constants, critical phase matching angle, and Θ_f [94Loi].

Sample	Na [mol%]	a [Å]	b [Å]	c [Å]	V [Å^3]	CPM [c]) angle	Θ_f [°C]
KTP	0	12.815	6.404	10.589	868.9	$\phi = 23.7°$	944 [a]) 957 [b])
KTP-006	4	12.811	6.402	10.592	868.7	–	956
KTP-007	7	12.792	6.392	10.589	865.8	–	949
KTP-008	18	12.787	6.384	10.585	864.0	$\phi = 19.8°$	–
KTP-010	47	12.734	6.367	10.574	857.3	$\theta = 12.7°$	914
KTP-015	13	–	–	–	865.5	$\phi = 22.4°$	–

[a]) HTS crystal.
[b]) Hydrothermal crystal.
[c]) CPM: critical phase matching.

Table 35B-1-006. $M_xM'_{1-x}TiOPO_4$ compounds. Lattice constants and SHG compared to that of quartz [89Phi].

Compound	*a* [Å]	*b* [Å]	*c* [Å]	*V* [Å^3]	SHG
$AgTiOPO_4$	12.524	6.263	10.53	825.95	5
$Ag_{0.87}K_{0.13}TiOPO_4$	12.534	6.294	10.524	830.23	7
$(NH_4)_{0.5}H_{0.5}TiOPO_4$	12.822	6.284	10.598	853.83	60
$KTiOPO_4$	12.816	6.403	10.587	868.68	6000
$(NH_4)_{0.5}K_{0.5}TiOPO_4$	12.894	6.442	10.58	878.81	1100
$TlTiOPO_4$	12.944	6.484	10.553	885.70	6000
$(NH_4)_{0.5}(H_3O)_{0.5}TiOPO_4$	12.915	6.495	10.589	888.18	700
NH_4TiOPO_4	12.916	6.492	10.598	888.62	2400
$RbTiOPO_4$	12.960	6.500	10.557	889.32	6000

Table 35B-1-007. $KTi_{1-x}V_xOPO_4$. Lattice parameters and SHG results [90Phi]. SHG intens: SHG intensity relative to KTP at λ = 1064 nm.

Compound	*a* [Å]	*b* [Å]	*c* [Å]	*V* [Å^3]	SHG intens (rel. to KTP)
$KTiOPO_4$	12.831(8)	6.415(2)	10.578(6)	870.7(8)	1.0
$KTi_{0.9975}V_{0.0025}OPO_4$	12.832(9)	6.414(4)	10.578(6)	870.6(9)	1.0
$KTi_{0.95}V_{0.05}OPO_4$	12.812(6)	6.412(7)	10.582(4)	869.2(10)	0.13
$KTi_{0.5}V_{0.5}OPO_4$	12.797(5)	6.397(6)	10.558(6)	864.2(10)	0.0008
$KVOPO_4$	12.779(9)	6.373(2)	10.510(2)	855.9(7)	–

Table 35B-1-008. $K_{0.84}(Ti_{0.92}Nb_{0.08})OPO_4$. Fractional coordinates and temperature parameters (in 10^{-4} Å^2 for cations, in 10^{-3} Å^2 for O atoms) [90Tho]. *B*: isotropic temperature parameter. For definitions of *B* and U_{ij}, see Eq. (e) and Eq. (d) in Introduction, respectively.

	x	*y*	*z*	Occupancy	*B* [Å^2]
K(1)	0.3791(1)	0.7813(2)	0.3103(0)	0.851(4)	1.51(4)
K(2)	0.1047(1)	0.6959(2)	0.0665(2)	0.840(4)	1.55(4)
Ti(1)	0.3725(1)	0.4995(1)	0.0008(1)	0.867(4)	0.45(2)
Nb(1)	0.3725(1)	0.4995(1)	0.0008(1)	0.133(4)	0.45(2)
Ti(2)	0.2473(0)	0.2659(1)	0.2513(1)	0.97(4)	0.47(4)
Nb(2)	0.2473(0)	0.2659(1)	0.2513(1)	0.03(4)	0.47(4)
P(1)	0.4984(1)	0.3373(2)	0.2586(3)	1.000(5)	0.44(3)
P(2)	0.1814(1)	0.5014(2)	0.5102(3)	1.000(6)	0.43(4)
O(1)	0.4862(4)	0.4848(7)	0.1463(5)	fixed	0.9(1)
O(2)	0.5103(4)	0.4678(9)	0.3806(5)	fixed	1.0(1)
O(3)	0.4007(3)	0.2000(7)	0.2778(5)	fixed	1.1(1)
O(4)	0.5942(3)	0.1934(6)	0.2389(5)	fixed	0.74(9)
OT(1)	0.2240(3)	0.9632(5)	0.6392(3)	fixed	0.63(9)
OT(2)	0.2241(4)	0.0420(8)	0.3867(4)	fixed	0.66(9)
O(5)	0.1119(3)	0.3133(7)	0.5392(4)	fixed	1.0(1)
O(6)	0.1122(3)	0.6928(7)	0.4843(5)	fixed	0.71(9)
O(7)	0.2529(4)	0.5414(8)	0.6249(5)	fixed	0.87(9)
O(8)	0.2541(4)	0.4620(8)	0.3973(4)	fixed	0.73(9)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
K(1)	262(7)	115(5)	227(8)	23(8)	76(5)	37(6)
K(2)	96(6)	236(7)	305(9)	4(7)	5(6)	74(5)
Ti/Nb(1)	46(4)	79(3)	33(4)	8(2)	–20(3)	–6(2)
Ti/Nb(2)	35(4)	105(4)	32(4)	38(3)	3(4)	3(2)
P(1)	24(8)	92(6)	27(8)	–6(8)	–4(5)	18(5)
P(2)	66(8)	80(7)	15(8)	–11(5)	10(7)	–5(3)
O(1)	3(2)	13(2)	10(2)	2(2)	–4(1)	–3(1)
O(2)	7(2)	11(2)	13(2)	–3(2)	1(1)	2(1)
O(3)	11(2)	13(2)	6(2)	–3(2)	–1(2)	0(1)
O(4)	2(2)	12(2)	7(2)	0(2)	2(1)	2(1)
OT(1) non-positive definite						
OT(2)	3(2)	13(2)	8(2)	3(2)	3(1)	–1(2)
O(5)	11(2)	99(2)	8(2)	2(1)	1(1)	–8(1)
O(6)	10(2)	13(2)	10(2)	–5(2)	–5(1)	–5(2)
O(7)	8(2)	12(2)	2(2)	–3(2)	–1(1)	–2(1)
O(8)	7(2)	11(2)	6(2)	–6(2)	2(1)	–3(2)

Table 35B-1-009. $K_{0.84}(Ti_{0.92}Nb_{0.08})OPO_4$. Comparison of bond-length statistics with that of KTP [90Tho].

	KTP	KTNP
Mean M–O bond lengths and average deviations from means *)		
Ti(1)–O	1.972(90)	1.973(87)
Ti(2)–O	1.967(79)	1.967(63)
K(1)–O	2.845(111)	2.854(124)
K(2)–O	2.934(127)	2.943(133)
Difference in K(1)–O means for KTP & KTNP	0.009	
Difference in K(2)–O means for KTP & KTNP	0.009	
Ti–OT–Ti chain-linking angles:		
OT(1)–Ti(1)–OT(2)	94.82°	95.21°
OT(2)–Ti(2)–OT(2)	175.14°	175.89°
Ti(2)–OT(1)–Ti(1)	135.99°	136.54°
Ti(1)–OT(2)–Ti(2)	133.36°	133.84°
Mean octahedral angles		
$Ti(1)O_6$ octahedron	89.78(4.36)°	89.83(4.23)°
$Ti(2)O_6$ octahedron	89.87(3.62)°	89.92(2.87)°

*) All bond lengths are given in Å.

Table 35B-1-010. $K_{0.5}Na_{0.5}TiOPO_4$. Atomic positions and isotropic temperature parameters (U_{iso}) [91Cre1]. For definition of temperature parameters, see Introduction.

	x	*y*	*z*	U_{iso} [$\cdot 10^{-2}$ Å^2]	Occupancy
Ti(1)	0.3721(2)	0.4911(8)	0.0000	0.37(6)	
Ti(2)	0.2489(4)	0.2699(7)	0.2515(7)	0.37(6)	
P(1)	0.4959(3)	0.3363(2)	0.2627(6)	0.47(3)	
P(2)	0.1839(1)	0.4998(7)	0.5123(6)	0.47(3)	
Na(1)	0.3528(3)	0.7689(7)	0.2898(6)	3.39(13)	0.96(7)
K(1)	0.3528(3)	0.7689(7)	0.2898(6)	3.41(12)	0.04(7)
Na(2)	0.1030(4)	0.6776(8)	0.0687(7)	3.39(13)	–0.05(8)
K(2)	0.1030(4)	0.6776(8)	0.0687(7)	3.41(13)	1.05(8)
O(1)	0.4810(2)	0.4939(5)	0.1521(5)	0.80(2)	
O(2)	0.5064(4)	0.4648(4)	0.3870(5)	0.80(2)	
O(3)	0.3997(2)	0.1898(4)	0.2782(6)	0.80(2)	
O(4)	0.5941(2)	0.1975(5)	0.2434(6)	0.80(2)	
O(5)	0.1171(3)	0.3031(4)	0.5377(5)	0.80(2)	
O(6)	0.1103(3)	0.6866(5)	0.4869(6)	0.80(2)	
O(7)	0.2556(3)	0.5290(6)	0.6275(6)	0.80(2)	
O(8)	0.2567(3)	0.4600(6)	0.3972(6)	0.80(2)	
O(9)	0.2253(3)	–0.0363(6)	0.6409(6)	0.80(2)	
O(10)	0.2242(3)	0.0296(6)	0.3855(6)	0.80(2)	

Table 35B-1-011. $Rb_{0.5}Na_{0.5}TiOPO_4$. Atomic positions and isotropic temperature parameters (U_{iso}) [91Cre1]. For definition of temperature parameters, see Introduction.

	x	*y*	*z*	U_{iso} [$\cdot 10^{-2}$ Å^2]	Occupancy
Ti(1)	0.3730(6)	0.4704(13)	0.0000	0.54(11)	
Ti(2)	0.2504(10)	0.2466(13)	0.2654(16)	0.54(11)	
P(1)	0.4959(5)	0.3349(7)	0.2660(11)	0.08(7)	
P(2)	0.1854(3)	0.4807(11)	0.5201(10)	0.08(7)	
Na(1)	0.3512(9)	0.7417(18)	0.2967(12)	3.02(15)	0.97(3)
Rb(1)	0.3512(9)	0.7417(18)	0.2967(12)	3.02(15)	0.03(3)
Na(2)	0.0988(5)	0.6613(10)	0.0745(10)	3.02(15)	0.04(3)
Rb(2)	0.0988(5)	0.6613(10)	0.0745(10)	3.02(15)	0.96(3)
O(1)	0.4856(5)	0.4750(10)	0.1490(10)	0.90(3)	
O(2)	0.5119(5)	0.4869(10)	0.3838(9)	0.90(3)	
O(3)	0.4037(6)	0.1856(8)	0.2900(10)	0.90(3)	
O(4)	0.5976(6)	0.2022(8)	0.2544(10)	0.90(3)	
O(5)	0.1222(5)	0.2875(8)	0.5446(9)	0.90(3)	
O(6)	0.1083(5)	0.6711(9)	0.4932(10)	0.90(3)	
O(7)	0.2520(5)	0.5177(9)	0.6394(9)	0.90(3)	
O(8)	0.2597(5)	0.4435(9)	0.4083(10)	0.90(3)	
O(9)	0.2193(5)	–0.0491(10)	0.6520(10)	0.90(3)	
O(10)	0.2280(6)	0.0139(9)	0.3956(9)	0.90(3)	

Table 35B-1-012. $K_{0.5}Na_{0.5}TiOPO_4$ (KNTP), $Rb_{0.5}Na_{0.5}TiOPO_4$ (RNTP). Selected bond lengths and angles with those of $KTiOPO_4$ (KTP) [91Cre1].

Bond	Bond length [Å]			Bond	Bond length [Å]		
	KNTP	RNTP	KTP		KNTP	RNTP	KTP
Ti(1)–O(1)	2.129(5)	2.14(1)	2.161(4)	Ti(2)–O(3)	2.010(6)	2.02(1)	2.037(3)
–O(2)	1.979(5)	1.95(1)	1.957(4)	–O(4)	1.988(6)	1.99(1)	1.979(3)
–O(5)	2.016(5)	2.06(1)	2.047(4)	–O(7)	2.012(6)	1.97(1)	1.966(4)
–O(6)	1.942(6)	1.91(1)	1.900(4)	–O(8)	1.959(6)	1.97(1)	1.994(4)
–O(9)	1.951(6)	2.00(1)	1.993(4)	–O(9)	1.728(6)	1.80(1)	1.738(4)
–O(10)	1.744(5)	1.73(1)	1.718(4)	–O(10)	2.103(6)	2.04(1)	2.101(4)
K(1)–O(1)	2.797(5)	2.88(1)	2.900(4)	K(2)–O(1)	2.741(6)	2.836(9)	2.679(4)
–O(2)	2.931(6)	2.78(1)	2.743(4)	–O(2)	2.992(5)	3.219(9)	2.979(4)
–O(3)	2.729(5)	2.89(1)	2.717(4)	–O(3)	3.082(6)	3.021(9)	3.046(4)
–O(5)	2.709(5)	2.71(1)	2.874(4)	–O(4)	3.010(5)	2.990(8)	3.125(4)
–O(7)	2.752(5)	2.76(1)	3.059(4)	–O(5)	2.829(6)	2.871(8)	2.799(4)
–O(8)	2.571(5)	2.52(1)	2.762(4)	–O(7)	2.928(6)	3.039(9)	2.917(4)
–O(9)	2.684(6)	2.56(1)	2.987(4)	–O(8)	3.114(6)	3.098(9)	3.044(4)
–O(10)	2.537(6)	2.56(1)	2.717(4)	–O(9)	2.685(7)	2.810(8)	2.765(4)
				–O(10)	3.083(6)	3.067(9)	3.055(4)
P(1)–O(1)	1.550(3)	1.531(3)	1.523(4)	P(2)–O(5)	1.531(3)	1.491(3)	1.541(4)
–O(2)	1.554(3)	1.591(3)	1.550(4)	–O(6)	1.532(3)	1.586(3)	1.533(4)
–O(3)	1.546(3)	1.536(3)	1.549(4)	–O(7)	1.537(3)	1.545(4)	1.551(4)
–O(4)	1.543(3)	1.557(3)	1.547(4)	–O(8)	1.554(3)	1.539(4)	1.543(4)

	Bond angle [°]		
	KNTP	RNTP	KTP
O(1)–P(1)–O(2)	108.5(1)	107.3(3)	108.7(2)
O(1)–P(1)–O(3)	111.6(3)	115.1(3)	112.3(2)
O(1)–P(1)–O(4)	111.4(3)	108.7(5)	110.8(2)
O(2)–P(1)–O(3)	106.9(3)	110.0(5)	105.8(2)
O(2)–P(1)–O(4)	109.9(3)	106.3(5)	110.2(2)
O(3)–P(1)–O(4)	108.6(1)	109.0(3)	108.8(2)
O(5)–P(2)–O(6)	108.4(1)	108.5(3)	109.4(2)
O(5)–P(2)–O(7)	106.8(3)	106.4(5)	107.8(2)
O(5)–P(2)–O(8)	109.8(3)	110.0(5)	111.2(2)
O(6)–P(2)–O(7)	114.3(3)	110.1(5)	111.2(2)
O(6)–P(2)–O(8)	110.7(3)	111.3(4)	110.4(2)
O(7)–P(2)–O(8)	106.7(1)	108.2(3)	106.7(2)

Table 35B-1-013. $K_{0.5}Rb_{0.5}TiOPO_4$. Selected bond distances [91Cre1]. The cation bond lengths are compared with those of $KTiOPO_4$ (KTP) and $RbTiOPO_4$ (RTP). Data of KTP and RTP are from [74Tor].

Bond	Bond length [Å]	Bond	Bond length [Å]
Ti(1)–O(1)	2.118(7)	Ti(2)–O(3)	2.028(9)
–O(2)	1.981(7)	–O(4)	2.016(9)
–O(5)	2.095(9)	–O(7)	2.029(9)
–O(6)	1.978(9)	–O(8)	1.917(10)
–O(9)	1.933(8)	–O(9)	1.757(9)
–O(10)	1.756(7)	–O(10)	2.085(9)

Bond	Bond length [Å]		
	KRTP	KTP	RTP
K(1)–O(1)	2.864(7)	2.900(4)	2.996
–O(2)	2.704(8)	2.743(4)	2.757
–O(3)	2.716(7)	2.717(4)	2.734
–O(5)	2.945(8)	2.874(4)	2.953
–O(7)	3.107(7)	3.059(4)	3.180
–O(8)	2.806(8)	2.762(4)	2.827
–O(9)	3.063(7)	2.987(4)	3.126
–O(10)	2.758(9)	2.717(4)	2.773
	KRTP	KTP	RTP
K(1)–O(1)	2.760(7)	2.679(4)	2.739
–O(2)	3.088(6)	2.979(4)	3.060
–O(3)	3.097(6)	3.046(4)	3.107
–O(4)	3.041(6)	3.125(4)	3.060
–O(5)	2.792(7)	2.799(4)	2.841
–O(7)	2.988(8)	2.917(4)	2.997
–O(8)	3.153(7)	3.044(4)	3.113
–O(9)	2.753(8)	2.765(4)	2.812
–O(10)	3.198(7)	3.055(4)	3.107

Table 35B-1-014. $K_{0.86}Rb_{0.14}TiOPO_4$ (flux grown), $K_{0.84}Rb_{0.16}TiOPO_4$ (ion-exchanged) [94Tho]. Atomic coordinates and equivalent temperature parameters U_{eq} [Å^2]. $U_{eq} = (U_{11} + U_{22} + U_{33})/3$.

	x	*y*	*z*	U_{eq}	Site occupancy
(1) Flux-grown $K_{0.86}Rb_{0.14}TiOPO_4$					
K(1)	0.37846(5)	0.77913(9)	0.68696(7)	0.0179(3)	
(K,Rb)(2)	0.10408(3)	0.69029(8)	0.93056(6)	0.0193(2)	K 0.714(3) Rb 0.286(3)
Ti(1)	0.37304(3)	0.49738(7)	0.00006(6)	0.0062(1)	
Ti(2)	0.24767(4)	0.26711(6)	0.74747(5)	0.0064(1)	
P(1)	0.49886(5)	0.33558(9)	0.73995(7)	0.0064(2)	
P(2)	0.18111(4)	0.50000(11)	0.48726(7)	0.0067(2)	
O(1)	0.4860(2)	0.4837(3)	0.8508(2)	0.0106(8)	
O(2)	0.5111(2)	0.4666(4)	0.6180(2)	0.0105(8)	
O(3)	0.4019(1)	0.1977(3)	0.7194(2)	0.0101(8)	
O(4)	0.5946(1)	0.1939(3)	0.7582(2)	0.0093(7)	
O(5)	0.1136(1)	0.3076(4)	0.4584(2)	0.0100(8)	
O(6)	0.1115(2)	0.6878(3)	0.5136(2)	0.0114(8)	
O(7)	0.2522(2)	0.5387(3)	0.3712(2)	0.0100(8)	
O(8)	0.2536(2)	0.4587(3)	0.6000(2)	0.0107(7)	
O(9)	0.2234(2)	0.9629(3)	0.3554(2)	0.0087(7)	
O(10)	0.2236(2)	0.0391(4)	0.6094(2)	0.0101(8)	
(2) Ion-exchanged $K_{0.84}Rb_{0.16}TiOPO_4$					
K(1)	0.3790(1)	0.7796(2)	0.6871(2)	0.0210(7)	K 0.962(3)
(K,Rb)(2)	0.1035(1)	0.6877(2)	0.9312(1)	0.0217(6)	K 0.718(7) Rb 0.282(7)
Rb(3)	0.099(2)	0.344(3)	0.041(1)	0.010(5)	Rb 0.038(3)
Ti(1)	0.37280(7)	0.4978(2)	–0.0003(2)	0.0056(4)	
Ti(2)	0.2480(1)	0.2671(2)	0.7467(2)	0.0063(3)	
P(1)	0.4992(2)	0.3363(2)	0.7390(2)	0.0065(6)	
P(2)	0.1814(1)	0.4992(3)	0.4869(2)	0.0068(5)	
O(1)	0.4871(4)	0.4838(9)	0.8512(4)	0.011(2)	
O(2)	0.5114(4)	0.4670(9)	0.6176(3)	0.014(2)	
O(3)	0.4016(4)	0.1985(7)	0.7193(4)	0.010(2)	
O(4)	0.5953(3)	0.1951(7)	0.7582(5)	0.009(2)	
O(5)	0.1124(4)	0.3089(8)	0.4583(4)	0.010(2)	
O(6)	0.1122(4)	0.6887(7)	0.5122(5)	0.012(2)	
O(7)	0.2529(5)	0.5395(8)	0.3710(4)	0.011(2)	
O(8)	0.2539(4)	0.4616(8)	0.5993(4)	0.010(2)	
O(9)	0.2242(4)	0.9625(7)	0.3567(4)	0.009(2)	
O(10)	0.2244(4)	0.0391(9)	0.6082(4)	0.011(2)	

Table 35B-1-015. $K_{0.86}Rb_{0.14}TiOPO_4$ (flux grown) (1), $K_{0.84}Rb_{0.16}TiOPO_4$ (ion-exchanged) (2). Bond length [$Å^2$] and bond angles [°] [94Tho].

	(1)	(2)		(1)	(2)
$Ti(1)O_6$ octahedron			Cage around *M*(1)		
Ti(1)–O(10^{i})	1.719(2)	1.719(5)	*M*(1)–O(3^{viii})	2.723(2)	2.724(5)
Ti(1)–O(2^{ii})	1.957(2)	1.957(5)	*M*(1)–O(10^{viii})	2.723(2)	2.723(6)
Ti(1)–O(9^{ii})	1.983(2)	1.974(5)	*M*(1)–O(2)	2.731(2)	2.731(6)
Ti(1)–O(6^{iii})	2.001(2)	1.996(5)	*M*(1)–O(8)	2.765(2)	2.759(5)
Ti(1)–O(5^{i})	2.044(2)	2.051(5)	*M*(1)–O(5^{vii})	2.887(2)	2.881(5)
Ti(1)–O(1^{iv})	2.148(2)	2.154(5)	*M*(1)–O(1)	2.918(2)	2.924(5)
			M(1)–O(9^{v})	3.002(2)	3.021(5)
$Ti(2)O_6$ octahedron			*M*(1)–O(7^{vii})	3.065(2)	3.074(5)
Ti(2)–O(9^{v})	1.738(2)	1.748(5)			
Ti(2)–O(7^{v})	1.965(2)	1.965(4)	Cage around *M*(2)		
Ti(2)–O(4^{vi})	1.986(2)	1.983(5)	*M*(2)–O(1^{ix})	2.718(2)	2.720(5)
Ti(2)–O(8)	1.990(2)	2.000(5)	*M*(2)–O(9^{v})	2.770(2)	2.761(5)
Ti(2)–O(3)	2.052(2)	2.044(5)	*M*(2)–O(5^{x})	2.813(2)	2.790(5)
Ti(2)–O(10)	2.091(2)	2.094(5)	*M*(2)–O(7^{vii})	2.966(2)	2.985(5)
Ti(1^{vii})–O(9)–Ti(2^{i})	136.2(1)	136.3(3)	*M*(2)–O(2^{vii})	3.045(2)	3.047(5)
Ti(1^{v})–O(10)–Ti(2)	133.4(1)	133.0(3)	*M*(2)–O(3^{vii})	3.060(2)	3.053(4)
			M(2)–O(4^{vi})	3.069(2)	3.065(5)
$P(1)O_4$ tetrahedron			*M*(2)–O(10^{vii})	3.071(2)	3.052(5)
P(1)–O(1)	1.519(2)	1.527(5)	*M*(2)–O(8^{vii})	3.087(2)	3.101(5)
P(1)–O(4)	1.542(2)	1.545(5)			
P(1)–O(3)	1.544(2)	1.549(5)	Cage around Rb(3)		
P(1)–O(2)	1.549(2)	1.543(4)	Rb(3)–O(10^{i})		2.69(2)
			Rb(3)–O(6^{xi})		2.74(2)
$P(2)O_4$ tetrahedron			Rb(3)–O(2^{iii})		2.92(2)
P(2)–O(6)	1.526(2)	1.530(5)	Rb(3)–O(3^{xi})		2.95(2)
P(2)–O(8)	1.537(2)	1.531(5)	Rb(3)–O(4^{xii})		3.01(2)
P(2)–O(5)	1.538(2)	1.539(5)	Rb(3)–O(9^{iii})		3.09(2)
P(2)–O(7)	1.552(2)	1.556(5)	Rb(3)–O(8^{iii})		3.16(2)
			Rb(3)–O(1^{xii})		3.25(2)
			Rb(3)–O(7^{iii})		3.27(2)

Symmetry codes: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x+1, -y+1, z-\frac{1}{2}$;
(iii) $-x+\frac{1}{2}, y-\frac{1}{2}, z-\frac{1}{2}$; (iv) $x, y, z-1$; (v) $-x+\frac{1}{2}, y-\frac{1}{2}, z+\frac{1}{2}$;
(vi) $x-\frac{1}{2}, -y+\frac{1}{2}, z$; (vii) $-x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}$; (viii) $x, y+1, z$; (ix) $x-\frac{1}{2}, -y+\frac{3}{2}, z$;
(x) $-x, -y+1, z+\frac{1}{2}$, (xi) $-x, -y+1, z-\frac{1}{2}$; (xii) $x-\frac{1}{2}, -y+\frac{1}{2}, z-1$.

Table 35B-1-016. $K_{0.59}Tl_{0.41}TiOPO_4$. Atomic coordinates, site occupancies q, and temperature parameters B [Å^2] [94Vor]. B: isotropic temperature parameters, for definition see Eq. (e) in Introduction.

Atom	x	y	z	q	B
Ti(1)	3724(1)	4968(1)	0	1.0	0.24(1)
Ti(2)	2478(1)	2668(1)	2528(1)	1.0	0.24(1)
P(1)	4991(1)	3358(1)	2603(1)	1.0	0.25(2)
P(2)	1816(1)	4999(2)	5129(1)	1.0	0.24(3)
K(1)	1028(1)	6925(1)	746(1)	0.379(1)	1.41(4)
Tl(1)	1028(1)	6925(1)	746(1)	0.621(1)	1.41(4)
K(2)	3822(1)	7838(1)	3238(1)	0.799(1)	1.93(4)
Tl(2)	3822(1)	7838(1)	3238(1)	0.201(1)	1.93(4)
O(1)	4861(2)	4829(5)	1482(3)	1.0	0.60(9)
O(2)	5111(2)	4662(5)	3821(2)	1.0	0.54(5)
O(3)	4018(2)	1986(4)	2800(3)	1.0	0.54(5)
O(4)	5956(2)	1956(4)	2426(2)	1.0	0.43(7)
O(5)	1147(2)	3068(4)	5404(3)	1.0	0.55(10)
O(6)	1126(2)	6899(4)	4857(3)	1.0	0.64(3)
O(7)	2524(2)	5393(4)	6288(3)	1.0	0.52(5)
O(8)	2540(2)	4577(5)	4001(3)	1.0	0.60(8)
O(9)	2237(2)	386(5)	3902(3)	1.0	0.52(4)
O(10)	2234(2)	373(4)	6444(3)	1.0	0.44(10)

Table 35B-1-017. $K_{0.59}Tl_{0.41}TiOPO_4$. Interatomic distances [Å] [94Vor].

P(1)–O(1)	1.527(1)	Ti(1)–O(9)	1.720(1)	K,Tl(1)–O(1)	2.688(1)	K,Tl(2)–O(2)	2.704(1)
P(1)–O(2)	1.546(1)	Ti(1)–O(10)	1.977(1)	K,Tl(1)–O(2)	3.066(1)	K,Tl(2)–O(3)	2.721(1)
P(1)–O(3)	1.547(1)	Ti(1)–O(5)	2.047(1)	K,Tl(1)–O(3)	3.120(1)	K,Tl(2)–O(5)	3.005(1)
P(1)–O(4)	1.546(1)	Ti(1)–O(6)	1.990(1)	K,Tl(1)–O(4)	3.068(1)	K,Tl(2)–O(7)	3.158(1)
P(2)–O(5)	1.540(1)	Ti(2)–O(3)	2.051(1)	K,Tl(1)–O(5)	2.824(1)	K,Tl(2)–O(8)	2.789(1)
P(2)–O(6)	1.538(1)	Ti(2)–O(4)	1.979(1)	K,Tl(1)–O(7)	2.965(1)	K,Tl(2)–O(9)	2.711(1)
P(2)–O(7)	1.550(1)	Ti(2)–O(9)	2.089(1)	K,Tl(1)–O(8)	3.119(1)	K,Tl(2)–O(10)	3.118(1)
P(2)–O(8)	1.540(1)	Ti(2)–O(10)	1.745(1)	K,Tl(1)–O(9)	3.128(1)		
Ti(1)–O(1)	2.148(1)	Ti(2)–O(7)	1.966(1)	K,Tl(1)–O(10)	2.784(1)		
Ti(1)–O(2)	1.967(1)	Ti(2)–O(8)	1.986(1)	K,Tl(2)–O(1)	2.999(1)		

Table 35B-1-018. $K_xRb_{1-x}TiOPO_4$, $KGeOPO_4$. Thermal expansion coefficients, elastic stiffnesses [4...50 MHz], thermoelastic stiffnesses $T_{\lambda\mu} = \mathrm{d}\ln c_{\lambda\mu}/\mathrm{d}T$ [94Hau]. T = 293 K.

	x = 1	x = 0.85	x = 0.7	$KGeOPO_4$
α_{11} [$\cdot 10^{-6}$ K^{-1}]	7.4(5)	9.5(6)	6.4(3)	13.3(8)
α_{22}	8.9(5)	9.8(6)	8.9(5)	18.2(6)
α_{33}	0.1(2)	0.3(2)	0.7(3)	–10.9(6)
c_{11} [$\cdot 10^{10}$ Nm^{-2}]	16.75(3)	16.55(3)	16.74(3)	17.38(3)
c_{22}	16.48(3)	16.31(3)	16.53(3)	16.81(3)
c_{33}^D	18.26(3)	18.05(3)	18.32(3)	23.40(3)
c_{44}^D	5.44(3)	5.34(3)	5.55(3)	6.48(3)
c_{55}^D	5.47(3)	5.46(3)	5.49(3)	6.26(3)
c_{66}	4.30(3)	4.34(3)	4.41(3)	5.81(3)
c_{12}	3.51(7)	3.14(7)	3.74(7)	5.76(7)
c_{13}	4.70(7)	4.19(7)	4.90(7)	6.09(7)
c_{23}	4.74(7)	4.61(7)	5.44(7)	8.43(7)
T_{11} [$\cdot 10^{-3}$ K^{-1}]	–0.18(1)	–0.16(2)	–0.15(1)	–0.21(3)
T_{22}	–0.17(1)	–0.15(2)	–0.15(1)	–0.33(4)
T_{33}^D	–0.15(1)	–0.16(2)	–0.13(1)	–0.22(3)
T_{44}^D	–0.36(3)	–0.20(3)	–0.22(2)	–0.21(3)
T_{55}^D	–0.26(3)	–0.37(3)	–0.16(2)	–0.31(5)
T_{66}	–0.27(3)	–0.15(3)	–0.12(2)	–0.09(2)
T_{12}	0.2(1)	0.1(1)	0.1(1)	0.1(1)
T_{13}	0.05(5)	0.1(1)	0.05(5)	0.2(1)
T_{23}	0.2(1)	0.0(1)	0.1(1)	0.1(1)

Table 35B-1-019. $K_{0.7}Rb_{0.3}TiOPO_4$. Dielectric constants as a function of frequency [94Wan].

Frequency [kHz]	κ_{11}	κ_{22}	κ_{33}
10	10.5(8)	10.6(1)	15.6(3)
20	10.5(5)	10.6(0)	15.6(4)
40	10.4(3)	10.6(1)	15.7(5)
100	10.6(0)	10.6(1)	15.6(4)
200	10.5(6)	10.6(0)	15.6(2)
400	10.5(6)	10.6(0)	15.3(9)
1000	10.6(2)	10.6(5)	15.5(8)
2000	10.8(1)	11.3(9)	15.9(9)
4000	10.4(6)	10.5(5)	15.0(0)
100000	10.4(5)	10.4(8)	14.5(2)

Table 35B-1-020. $K_xRb_{1-x}TiOPO_4$, $KGeOPO_4$, $KTiOAsO_4$. Lattice constants, density, dielectric constants, refractive indices [94Hau]. $T = 293$ K.

		x = 1	x = 0.85	x = 0.75	x = 0.7	$KGeOPO_4$	$KTiOAsO_4$
a_1	[Å]	12.823(3)	12.833(4)	12.839(2)	12.840(8)	12.604(3)	13.129(8)
a_2	[Å]	6.407(2)	6.410(2)	6.411(2)	6.460(3)	6.302(2)	6.577(8)
a_3	[Å]	10.604(3)	10.600(2)	10.605(1)	10.610(5)	10.016(3)	10.786(4)
ρ	[10^3 kg m^{-3}]	3.055(2)	3.089(4)	3.160(7)	3.206(2)	3.433(4)	
κ_{11}	20 kHz	10.4(1)	10.6(1)	10.7(1)	10.6(1)	9.1(2)	
	100 kHz	10.4(1)	10.0(1)	10.0(1)	10.6(1)	8.6(2)	
	1 MHz	10.5(1)	10.2(1)	10.1(1)	10.6(1)	8.3(2)	
	100 MHz	10.7(1)	10.1(1)	10.2(1)	10.5(1)	8.4(2)	
κ_{22}	10 kHz	10.3(1)	10.0(1)	9.6(1)	10.6(1)	7.8(2)	
	100 kHz	10.0(1)	10.0(1)	9.3(1)	10.6(1)	7.7(2)	
	1 MHz	10.0(1)	10.0(1)	9.0(1)	10.7(1)	7.6(2)	
	100 MHz	10.4(1)	10.0(1)	9.1(1)	10.5(1)	7.7(2)	
κ_{33}	20 kHz	46.0(2)	14.8(6)	14.5(6)	15.6(6)	18.5(7)	
	100 kHz	21.2(7)	13.9(5)	14.2(6)	15.6(6)	18.1(4)	
	1 MHz	12.7(7)	13.0(5)	12.9(5)	15.6(5)	17.6(6)	
	100 MHz	11.6(5)	13.2(5)	14.5(5)	14.5(5)	17.9(6)	
n_1	420 nm	1.8119(1)	1.8182(3)	1.8203(8)	1.8215(3)	1.6753(3)	1.8635(5)
	500 nm	1.791(1)	1.7892(2)	1.7914(7)	1.7921(3)	1.6652(3)	1.8328(5)
	600 nm	1.770(1)	1.7704(4)	1.7723(2)	1.7726(3)	1.6580(3)	1.8125(5)
	680 nm	1.760(1)	1.7618(5)	1.7633(4)	1.7635(4)	1.6542(3)	1.8025(2)
n_2	420 nm	1.829(1)	1.8303(3)	1.8334(9)	1.8347(3)	1.6802(3)	1.8804(7)
	500 nm	1.797(1)	1.7980(6)	1.8008(2)	1.8017(3)	1.6704(3)	1.8435(2)
	600 nm	1.775(1)	1.7778(9)	1.7796(7)	1.7804(3)	1.6631(5)	1.8115(5)
	680 nm	1.764(1)	1.7677(5)	1.7703(5)	1.7705(4)	1.6593(5)	1.8093(5)
n_3	420 nm	1.949(1)	1.9520(3)	1.953(1)	1.9530(3)	1.6914(9)	2.0019(4)
	500 nm	1.901(1)	1.9032(2)	1.9053(2)	1.9069(3)	1.6807(7)	1.9489(5)
	600 nm	1.871(1)	1.8736(9)	1.8754(7)	1.8765(4)	1.6728(9)	1.9162(9)
	680 nm	1.858(1)	1.8604(5)	1.8623(5)	1.8628(4)	1.6684(9)	1.9016(8)

Table 35B-1-021. $K_{0.7}Rb_{0.3}TiOPO_4$. Coefficients for Sellmeier equation, $n^2 = A + B/(1 - C\lambda^2) - D\lambda^2$ [94Wan]. λ: wave length [μm].

	A	*B*	*C*	*D*
n_x	2.178669	0.845917	0.046031	0.017280
n_y	2.206336	0.841677	0.049316	0.017298
n_z	2.257201	1.080122	0.054277	0.021782

Table 35B-1-022. $K_{0.85}Rb_{0.15}TiOPO_4$. Sellmeier coefficients for describing the optical dispersion at 293 K [94Hau]. $n^2 = A + B/(1 - C\lambda^2) - D\lambda^2$; λ: wave length in vacuum [μm].

	A	*B*	*C*	*D*
n_1	2.17130	0.84343	0.04610	0.01724
n_2	2.20316	0.83611	0.04953	0.01726
n_3	2.25447	1.07465	0.05460	0.02174

Table 35B-1-023. $K_{0.7}Rb_{0.3}TiOPO_4$. Piezooptic constants [94Wan].

Π_{11}	+2.79(3)
Π_{22}	+1.800(25)
Π_{33}	+4.940(24)
Π_{44}	–8.80(25)
Π_{55}	–4.720(25)
Π_{66}	+6.320(25)
Π_{12}	+1.980(27)
Π_{13}	+3.260(37)
Π_{23}	+7.35(2)
Π_{21}	+4.32(2)
Π_{31}	+3.200(25)
Π_{32}	–1.450(26)

Table 35B-1-024. $K_{0.5}Na_{0.5}TiOPO_4$, $Rb_{0.5}Na_{0.5}TiOPO_4$. Quadrupole coupling constants e^2qQ/h and asymmetry parameters η of ^{23}Na nuclei [91Cre1].

Material	e^2qQ/h [MHz]	η
$K_{0.5}Na_{0.5}TiOPO_4$	1.75	0.40
$Rb_{0.5}Na_{0.5}TiOPO_4$	1.7	0.47