

Table 35A-6-001. KTiOPO₄, RbTiOPO₄, TlTiOPO₄. Unit cell parameters [71Mas]. σ : standard deviation.

	a [Å]	b [Å]	c [Å]	V [Å ³]	ρ_x [$\cdot 10^3$ kg m ⁻³]	ρ_m [$\cdot 10^3$ kg m ⁻³]
KTiOPO ₄	12.814	6.404	10.616	871.1	3.019	3.00
RbTiOPO ₄	12.971	6.492	10.577	890.7	3.638	
TlTiOPO ₄	12.983	6.490	10.578	891.3	5.409	
σ	0.006	0.002	0.005	1.0	0.005	

Table 35A-6-002. KTiOPO₄. Lattice constants of crystals of different origins [86Bal].

Hydrothermal method	$a = 12.800$ Å $b = 6.400$ Å $c = 10.580$ Å
Flux method	$a = 12.840$ Å $b = 6.396$ Å $c = 10.584$ Å

Table 35A-6-003. KTiOPO₄. Lattice parameters and unit cell volume of the non-irradiated, electron-irradiated and fast-neutron-irradiated crystals [91And]. Electron irradiation dose: $1 \cdot 10^6$ Gy. Neutron irradiation dose: $1 \cdot 10^{10}$ Gy.

Non-irradiated crystal	Irradiated by electrons	Irradiated by fast neutrons
$a = 12.8172(8)$ Å	$a = 12.8167(13)$ Å	$a = 12.8266(7)$ Å
$b = 6.4029(5)$ Å	$b = 6.4038(4)$ Å	$b = 6.4093(4)$ Å
$c = 10.5885(9)$ Å	$c = 10.5889(8)$ Å	$c = 10.5865(5)$ Å
$V = 868.967$ Å ³	$V = 869.085$ Å ³	$V = 870.314$ Å ³

Table 35A-6-004. KTiOPO₄. Unit cell dimensions and volume as functions of pressure [91All]. AP: atmospheric pressure.

Pressure [GPa]	AP	0.2	2.2	3.7	4.7	6.2
a [Å]	12.819(3)	12.832(7)	12.705(7)	12.639(7)	12.620(8)	12.477(9)
b [Å]	6.399(1)	6.412(3)	6.363(2)	6.331(2)	6.315(4)	6.322(3)
c [Å]	10.584(2)	10.586(4)	10.505(4)	10.447(4)	10.417(5)	10.058(4)
V [Å ³]	868.2(4)	871(1)	849(1)	836(1)	830(1)	793(1)

Table 35A-6-005. KTiOPO₄. Atomic coordinates and U_{ij} [\AA^2] [91Han]. For definition of U_{ij} , see Eq. (d) in Introduction.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti(1)	37293(1)	50001(2)	0	493(3)	453(3)	426(3)	−13(3)	−27(3)	61(3)
O(T2)	27623(4)	54109(9)	−11024(5)	825(16)	824(16)	747(15)	−67(14)	−292(13)	170(13)
Ti(2)	24666(1)	26941(2)	25129(2)	453(3)	501(3)	402(3)	−27(3)	51(3)	−12(3)
O(T1)	27529(4)	46681(8)	14324(5)	755(16)	789(16)	688(15)	39(13)	207(12)	228(13)
P(1)	49805(1)	33625(2)	25987(2)	367(4)	538(5)	478(5)	−4(4)	−68(4)	24(4)
O(1)	48570(4)	48655(8)	14995(2)	822(15)	963(17)	786(14)	−150(13)	−209(12)	388(13)
O(2)	50992(4)	46518(9)	38292(5)	766(15)	1018(16)	767(15)	132(13)	−268(12)	−324(13)
O(3)	40031(4)	19910(8)	27915(5)	443(13)	754(14)	959(15)	−117(11)	27(11)	105(12)
O(4)	59353(4)	19344(8)	24046(5)	442(12)	866(14)	1094(17)	140(11)	10(11)	−91(13)
P(2)	18083(1)	50209(3)	51241(2)	614(5)	390(4)	435(5)	−27(4)	33(4)	−65(4)
O(5)	11248(4)	31096(8)	54089(5)	910(15)	464(13)	955(16)	−134(12)	208(12)	3(11)
O(6)	11145(4)	69164(8)	48694(5)	1054(16)	473(13)	1123(18)	134(12)	−218(13)	21(12)
O(7)	25276(4)	53953(8)	62766(5)	947(16)	891(16)	707(14)	203(14)	−270(13)	−336(12)
O(8)	25294(4)	46089(9)	39915(5)	1007(17)	959(16)	675(14)	−263(14)	339(12)	−331(12)
K(1)	37709(6)	77988(7)	31023(8)	2266(18)	1028(13)	2024(18)	433(15)	551(17)	104(14)
K(2)	10569(4)	70040(10)	6486(8)	1264(15)	2047(19)	2338(20)	516(14)	−16(16)	−141(19)

Table 35A-6-006. KTP-type crystals. Comparison of bridging Ti–O distances in KTP-type structures [89Phi]. ΔTi : difference between two Ti–O distances.

	KTiOPO ₄	NaTiOPO ₄	NH ₄ TiOPO ₄	(NH ₄) _{0.5} (H ₃ O) _{0.5} TiOPO ₄
Ti(1)–O(9)	1.993 Å	1.958 Å	2.012 Å	2.155 Å
Ti(1)–O(10)	1.718 Å	1.719 Å	1.901 Å	1.788 Å
$\Delta\text{Ti}(1)$	0.275 Å	0.239 Å	0.111 Å	0.367 Å
Ti(2)–O(9)	1.738 Å	1.748 Å	2.116 Å	1.704 Å
Ti(2)–O(10)	2.101 Å	2.090 Å	1.763 Å	2.041 Å
$\Delta\text{Ti}(2)$	0.363 Å	0.342 Å	0.353 Å	0.337 Å

Table 35A-6-007. KTP-family crystals. Average trans Ti–O distances (R_{av}) and bond length differences (Δ_{Ti}) [90Phi].

Compound	$R_{av}(Ti(1))$ [Å]	$\Delta_{Ti(1)}$ [Å]	$R_{av}(Ti(2))$ [Å]	$\Delta_{Ti(2)}$ [Å]
KTiOPO ₄	1.940(6)	0.443(6)	1.920(6)	0.363(6)
KVOPO ₄	1.88(1)	0.42(1)	1.94(1)	0.53(1)
NH ₄ TiOPO ₄	1.932(5)	0.438(5)	1.919(6)	0.354(6)
TiTiOPO ₄	1.940(7)	0.429(7)	1.912(7)	0.329(7)
RbTiOPO ₄	1.940(6)	0.426(7)	1.922(7)	0.344(7)
AgTiOPO ₄	1.97(2)	0.52(2)	1.93(2)	0.29(2)
β -NaTiOPO ₄	1.972(8)	0.515(8)	1.929(8)	0.347(8)
(NH ₄) _{0.5} H _{0.5} TiOPO ₄	1.924(6)	0.046(6)	1.939(7)	–0.350(7)
(NH ₄) _{0.5} (H ₃ O) _{0.5} TiOPO ₄	1.92(4)	0.45(4)	1.92(3)	0.25(3)
KTiOAsO ₄	1.94(2)	0.40(2)	1.93(3)	0.33(3)
KTiO(PO ₄) _{0.5} (AsO ₄) _{0.5}	1.94(1)	0.43(1)	1.93(1)	0.33(1)
K _{0.5} (NH ₄) _{0.5} TiOAsO ₄	1.94(2)	0.42(2)	1.94(2)	0.36(2)
KGaPO ₄ F _{0.7} (OH) _{0.3}	1.928(8)	–0.027(8)	1.953(8)	0.056(8)
TiTiOPO ₄ (650 °C)	1.94(1)	0.23(1)	1.90(1)	0.00(1)
KSnOPO ₄	2.04(1)	0.14(1)	1.97(1)	0.01(1)

Table 35A-6-008. KTiOPO₄. Bond lengths of non-irradiated, electron-irradiated and fast-neutron-irradiated crystals [91And]. Electron irradiation dose: $1 \cdot 10^6$ Gy. Neutron irradiation dose: $1 \cdot 10^{10}$ Gy.

	non-irradiated crystal	irradiated by electrons	irradiated by fast neutrons
P(1)–O(1)	1.518(1) Å	1.518(1) Å	1.519(1) Å
P(1)–O(2)	1.551(1) Å	1.551(1) Å	1.551(1) Å
P(1)–O(3)	1.546(1) Å	1.544(1) Å	1.544(1) Å
P(1)–O(4)	1.541(1) Å	1.541(1) Å	1.541(1) Å
P(2)–O(5)	1.538(1) Å	1.537(1) Å	1.536(1) Å
P(2)–O(6)	1.529(1) Å	1.530(1) Å	1.528(1) Å
P(2)–O(7)	1.550(1) Å	1.549(1) Å	1.549(1) Å
P(2)–O(8)	1.535(1) Å	1.534(1) Å	1.535(1) Å
Ti(1)–O(1)	2.154(1) Å	2.155(1) Å	2.148(1) Å
Ti(1)–O(2)	1.955(1) Å	1.955(1) Å	1.959(1) Å
Ti(1)–O(Ti2)	1.985(1) Å	1.985(1) Å	1.976(1) Å
Ti(1)–O(Ti1)	1.716(1) Å	1.715(1) Å	1.723(1) Å
Ti(1)–O(5)	2.046(1) Å	2.048(1) Å	2.048(1) Å
Ti(1)–O(6)	1.987(1) Å	1.988(1) Å	1.988(1) Å
Ti(2)–O(3)	2.042(1) Å	2.044(1) Å	2.044(1) Å
Ti(2)–O(4)	1.980(1) Å	1.979(1) Å	1.979(1) Å
Ti(2)–O(Ti2)	1.736(1) Å	1.736(1) Å	1.744(1) Å
Ti(2)–O(Ti1)	2.099(1) Å	2.099(1) Å	2.087(1) Å
Ti(2)–O(7)	1.964(1) Å	1.965(1) Å	1.962(1) Å
Ti(2)–O(8)	1.998(1) Å	1.998(1) Å	1.996(1) Å

Table 35A-6-009. KTiOPO₄. Unit-cell dimensions [Å], unit-cell volume [Å³] and refined atomic fractional coordinates of KTiOPO₄ as a function of pressure [92All]. AP: atmospheric pressure. N_i : the number of independent reflections. N_r : the number of refined parameters. R_w : the weighted R factors.

		Pressure				
		AP	0.2 GPa	2.2 GPa	3.7 GPa	4.7 GPa
	a [Å]	12.819(3)	12.832(7)	12.705(7)	12.639(7)	12.620(8)
	b [Å]	6.399(1)	6.412(3)	6.363(2)	6.331(2)	6.315(4)
	c [Å]	10.584(2)	10.586(4)	10.505(4)	10.447(4)	10.417(5)
	V [Å ³]	868.1(4)	871(1)	849(1)	836(1)	830(1)
K(1)	x	0.37807(8)	0.3795(5)	0.3813(5)	0.3815(5)	0.3818(4)
	y	0.7806(1)	0.7799(5)	0.7796(5)	0.7807(5)	0.7819(5)
	z	0.6880(1)	0.6867(4)	0.6860(4)	0.6855(4)	0.6853(5)
K(2)	x	0.10526(7)	0.1049(6)	0.1049(6)	0.1045(5)	0.1046(4)
	y	0.6990(1)	0.6989(5)	0.6946(5)	0.6921(4)	0.6911(5)
	z	0.9332(1)	0.9331(6)	0.9325(5)	0.9332(5)	0.9320(6)
Ti(1)	x	0.37290(4)	0.3737(4)	0.3728(3)	0.3733(3)	0.3743(3)
	y	0.5001(1)	0.5013(5)	0.5004(4)	0.5013(4)	0.5006(4)
	z	−0.00040(8)	−0.0004	−0.0004	−0.0004	−0.0004
Ti(2)	x	0.24658(6)	0.2450(6)	0.2450(5)	0.2467(5)	0.2461(4)
	y	0.2695(5)	0.2697(4)	0.2690(4)	0.2686(3)	0.2685(3)
	z	0.74836(9)	0.7483(5)	0.7480(5)	0.7484(5)	0.7486(6)
P(1)	x	0.49808(8)	0.4986(8)	0.4981(8)	0.4980(7)	0.4970(6)
	y	0.3363(1)	0.3360(4)	0.3338(4)	0.3318(4)	0.3318(4)
	z	0.7397(1)	0.7409(6)	0.7419(6)	0.7409(5)	0.7404(6)
P(2)	x	0.18079(7)	0.1822(6)	0.1815(6)	0.1805(5)	0.1797(5)
	y	0.5020(1)	0.5000(9)	0.5003(7)	0.5029(8)	0.5024(6)
	z	0.4872(1)	0.4882(6)	0.4874(5)	0.4882(5)	0.4891(6)
O(1)	x	0.4859(2)	0.4852(14)	0.4873(12)	0.4868(13)	0.4890(12)
	y	0.4867(5)	0.4894(12)	0.4863(12)	0.4873(12)	0.4857(13)
	z	0.8497(2)	0.8478(9)	0.8522(8)	0.8500(9)	0.8481(11)
O(2)	x	0.5103(2)	0.5142(17)	0.5087(13)	0.5094(14)	0.5100(10)
	y	0.4657(5)	0.4616(12)	0.4604(12)	0.4583(13)	0.4600(13)
	z	0.6170(2)	0.6168(8)	0.6146(8)	0.6162(8)	0.6174(11)
O(3)	x	0.4004(2)	0.4009(12)	0.4023(12)	0.4009(12)	0.4004(9)
	y	0.1986(4)	0.2037(13)	0.1981(14)	0.1920(14)	0.1897(13)
	z	0.7208(2)	0.7192(10)	0.7234(9)	0.7226(10)	0.7272(13)
O(4)	x	0.5934(2)	0.5908(15)	0.5929(14)	0.5918(14)	0.5917(11)
	y	0.1930(4)	0.1888(13)	0.1851(13)	0.1836(13)	0.1840(14)
	z	0.7589(2)	0.7572(9)	0.7590(9)	0.7583(10)	0.7574(11)
O(T1)	x	0.2248(1)	0.2226(14)	0.2233(14)	0.2273(13)	0.2274(12)
	y	0.9653(4)	0.9694(16)	0.9714(15)	0.9737(14)	0.9703(15)
	z	0.3561(2)	0.3537(10)	0.3537(9)	0.3354(9)	0.3566(11)
O(T2)	x	0.2232(2)	0.2195(17)	0.2205(14)	0.2218(14)	0.2219(12)
	y	0.0413(5)	0.0423(18)	0.0388(17)	0.0428(15)	0.0407(15)
	z	0.6097(2)	0.6088(12)	0.6097(11)	0.6119(10)	0.6126(11)

(continued)

Table 35A-6-009 (continued)

		Pressure				
		AP	0.2 GPa	2.2 GPa	3.7 GPa	4.7 GPa
O(5)	<i>x</i>	0.1126(2)	0.1118(14)	0.1089(14)	0.1126(11)	0.1094(10)
	<i>y</i>	0.3106(4)	0.3162(13)	0.3141(12)	0.3177(12)	0.3143(12)
	<i>z</i>	0.4585(2)	0.4560(10)	0.4545(9)	0.4574(10)	0.4594(15)
O(6)	<i>x</i>	0.1113(2)	0.1119(15)	0.1120(15)	0.1087(15)	0.1083(13)
	<i>y</i>	0.6918(4)	0.6938(13)	0.6904(12)	0.6961(12)	0.6937(13)
	<i>z</i>	0.5117(3)	0.5129(11)	0.5127(9)	0.5124(10)	0.5126(12)
O(7)	<i>x</i>	0.2525(2)	0.2506(17)	0.2551(17)	0.2575(15)	0.2560(13)
	<i>y</i>	0.5402(5)	0.5420(16)	0.5415(15)	0.5364(15)	0.5419(15)
	<i>z</i>	0.3718(2)	0.3713(10)	0.3720(9)	0.3734(10)	0.3747(11)
O(8)	<i>x</i>	0.2528(2)	0.2522(14)	0.2560(11)	0.2542(12)	0.2536(12)
	<i>y</i>	0.4619(5)	0.4598(16)	0.4598(14)	0.4602(15)	0.4602(16)
	<i>z</i>	0.6008(2)	0.6014(12)	0.6003(10)	0.6015(11)	0.6006(12)
	<i>N_i</i>	2158	490	491	496	417
	<i>N_r</i>	145	65	65	65	65
	<i>R_w</i>	0.024	0.044	0.042	0.047	0.051

Table 35A-6-010. KTiOPO₄. Bond lengths [Å] of the K cages, Ti octahedra and P tetrahedra as a function of pressure [92All]. The atmospheric-pressure (AP) values were taken from [90Tho].

		Pressure				
		AP	0.2 GPa	2.2 GPa	3.7 GPa	4.7 GPa
K(1)O ₈	K1–O1	2.894(4)	2.867(12)	2.889(11)	2.859(11)	2.865(12)
	K1–O2	2.738(4)	2.775(16)	2.703(13)	2.702(14)	2.693(12)
	K1–O3	2.712(3)	2.753(10)	2.705(10)	2.644(10)	2.622(10)
	K1–O5	2.872(3)	2.862(10)	2.832(9)	2.851(10)	2.864(15)
	K1–O7	3.057(3)	3.071(14)	3.099(15)	3.092(12)	3.100(13)
	K1–O8	2.755(4)	2.774(15)	2.736(11)	2.734(13)	2.743(13)
	K1–OT1	2.995(3)	2.967(12)	2.953(12)	2.969(11)	2.992(12)
	K1–OT2	2.722(4)	2.780(19)	2.745(16)	2.724(16)	2.705(13)
K(2)O ₉	K2–O1	2.677(3)	2.677(12)	2.658(12)	2.663(15)	2.656(11)
	K2–O2	2.982(3)	2.991(14)	2.933(11)	2.927(12)	2.950(12)
	K2–O3	3.045(3)	3.029(11)	3.057(10)	3.024(11)	3.075(12)
	K2–O4	3.117(3)	3.112(9)	3.031(8)	3.003(9)	2.991(10)
	K2–O5	2.806(3)	2.793(19)	2.727(18)	2.757(16)	2.717(14)
	K2–O7	2.918(4)	2.951(15)	2.905(14)	2.861(14)	2.891(13)
	K2–O8	3.048(4)	3.055(16)	3.013(14)	3.027(14)	3.028(14)
	K2–OT1	2.765(4)	2.789(15)	2.733(15)	2.663(15)	2.656(15)
Ti(1)O ₆	Ti1–O1	2.150(3)	2.153(13)	2.126(12)	2.123(13)	2.144(14)
	Ti1–O2	1.958(3)	1.915(17)	1.946(14)	1.936(15)	1.923(13)
	Ti1–O5	2.042(3)	2.079(8)	2.065(8)	2.058(8)	2.035(9)
	Ti1–O6	1.987(3)	1.985(8)	1.986(8)	1.950(8)	1.956(9)
	Ti1–OT1	1.981(3)	1.988(14)	1.968(13)	1.978(13)	1.975(13)
	Ti1–OT2	1.716(3)	1.684(17)	1.675(13)	1.700(13)	1.710(13)
Ti(2)O ₆	Ti2–O3	2.044(3)	2.067(15)	2.065(16)	2.026(15)	2.022(11)
	Ti2–O4	1.981(3)	1.999(16)	1.958(17)	1.983(17)	1.974(13)
	Ti2–O7	1.965(3)	1.957(11)	1.948(10)	1.967(10)	1.942(10)
	Ti2–O8	1.990(3)	1.978(11)	1.975(10)	1.958(10)	1.963(11)
	Ti2–OT1	1.733(3)	1.749(12)	1.748(10)	1.745(10)	1.732(11)
	Ti2–OT2	2.092(3)	2.101(12)	2.086(11)	2.043(11)	2.042(11)
P(1)O ₄	P1–O1	1.519(3)	1.509(10)	1.517(9)	1.513(9)	1.489(12)
	P1–O2	1.548(3)	1.554(9)	1.567(9)	1.537(9)	1.525(12)
	P1–O3	1.544(3)	1.531(15)	1.505(15)	1.525(14)	1.520(12)
	P1–O4	1.541(3)	1.523(17)	1.542(18)	1.523(17)	1.527(13)
P(2)O ₄	P2–O5	1.535(3)	1.523(15)	1.540(14)	1.488(13)	1.515(10)
	P2–O6	1.528(3)	1.557(14)	1.521(15)	1.544(15)	1.526(12)
	P2–O7	1.548(3)	1.541(15)	1.553(16)	1.559(14)	1.553(14)
	P2–O8	1.537(3)	1.520(13)	1.539(12)	1.530(13)	1.513(13)

Table 35A-6-011. KTiOPO₄. Pressure dependence of the average M–O bond lengths [Å] in the TiO₆ octahedra, PO₄ tetrahedra, K cages and of the volumes [Å³] of these structural units [92All]. The atmospheric-pressure (AP) values are taken from [90Tho].

	Pressure				
	AP	0.2 GPa	2.2 GPa	3.7 GPa	4.7 GPa
TiO ₆ octahedra					
Average bond length [Å]	1.970(3)	1.971(13)	1.962(12)	1.956(12)	1.952(12)
Volume [Å ³]	10.08(5)	10.08(18)	9.94(17)	9.86(17)	9.80(16)
PO ₄ tetrahedra					
Average bond length [Å]	1.537(3)	1.532(13)	1.534(13)	1.527(13)	1.521(12)
Volume [Å ³]	1.86(1)	1.84(5)	1.86(5)	1.83(5)	1.80(4)
K1 cage					
Average bond length [Å]	2.843(4)	2.856(14)	2.833(12)	2.822(12)	2.823(12)
Volume [Å ³]	26.15(6)	26.46(36)	25.72(33)	25.14(34)	25.00(31)
K2 cage					
Average bond length [Å]	2.934(3)	2.943(15)	2.902(13)	2.884(14)	2.889(13)
Volume [Å ³]	34.71(7)	35.12(45)	33.46(45)	32.91(45)	33.03(45)

Table 35A-6-012. KTiOPO₄, RbTiOPO₄, TiTiOPO₄, $c_{\lambda\lambda}$ [$\cdot 10^9$ N m⁻²], determined by Brillouin scattering [89Ale].

	KTiOPO ₄	RbTiOPO ₄	TiTiOPO ₄
c_{11}	159(3)	143(3)	155(5)
c_{22}	154(3)	142(3)	154(5)
c_{33}	175(3)	175(3)	161(5)
c_{44}	—	33(3)	—
c_{55}	—	40(8)	—
c_{66}	—	57(9)	—

Table 35A-6-013. KTiOPO₄, RbTiOPO₄, KTiOAsO₄, RbTiOAsO₄, CsTiOAsO₄. Sellmeier coefficients for the principal refractive indices of KTP isomorphs [94Che1]. (Sellmeier equation: $n_i(\lambda)^2 = A_i + B_i [1 - (C_i/\lambda)^2]^{-1} - D_i \lambda^2$, $i = x, y, z$).

Crystal	A_x	B_x	C_x [μm]	D_x [μm^{-2}]	A_y	B_y	C_y [μm]	D_y [μm^{-2}]	A_z	B_z	C_z [μm]	D_z [μm^{-2}]
KTiOPO ₄	2.11460	0.89188	0.20861	0.01320	2.15180	0.87862	0.21801	0.01327	2.31360	1.00012	0.23831	0.01679
RbTiOPO ₄	2.15559	0.93307	0.20994	0.01452	2.38494	0.73603	0.23891	0.01583	2.27723	1.11030	0.23454	0.01995
KTiOAsO ₄	2.11055	1.03177	0.21088	0.01064	2.38888	0.77900	0.23784	0.01501	2.34723	1.10111	0.24016	0.01739
RbTiOAsO ₄	2.22681	0.99616	0.21433	0.01369	1.97756	1.25726	0.20448	0.00865	2.28779	1.20629	0.23484	0.01583
CsTiOAsO ₄	2.34498	1.04863	0.22044	0.01483	2.74440	0.70733	0.26033	0.01526	2.53666	1.10600	0.24988	0.01711

Table 35A-6-014. KTiOPO₄. Constants for Sellmeier equations [88Dya]. Sellmeier equation: $n(\lambda)^2 = A + B/(1 - C\lambda^{-2}) - D\lambda^2$.

n	A	B	C [10 ⁻¹² m ²]	D [10 ¹² m ⁻²]
n_x	2.10468	0.89342	0.04438	0.01036
n_y	2.14559	0.87629	0.04850	0.01173
n_z	1.94460	1.36170	0.04700	0.01491

Table 35A-6-015. KTiOPO₄. OH⁻ and OD⁻ vibrational frequencies [cm⁻¹] measured by IR absorption [86Ahm]. The crystals were prepared by hydrothermal and flux methods using ordinary and heavy waters in separate runs.

¹⁶ OH ⁻ [cm ⁻¹]	¹⁶ OD ⁻ [cm ⁻¹]	Ratio
3602	2657	0.7376
3586	2646	0.7379
3582	2642	0.7376
3573	2610	0.7305
3566	2604	0.7302

Table 35A-6-016. KTiOPO₄. $r_{\lambda i}$, κ'_{ii} [89Bie]. $r_{\lambda i}$: electrooptic coefficients. Low frequency: kHz ... MHz range. High frequency: GHz range.

Constant	Low Frequency	High Frequency
r_{13} [pm V ⁻¹]	+9.5	+8.8
r_{23} [pm V ⁻¹]	+15.7	+13.8
r_{33} [pm V ⁻¹]	+36.3	+35.0
r'_{51} [pm V ⁻¹]	7.3	6.9
r'_{42} [pm V ⁻¹]	9.3	8.8
r_{e1} [pm V ⁻¹]	+28.6	+27.0
r_{e2} [pm V ⁻¹]	+22.2	+21.5
κ'_{11}	11.9	11.6
κ'_{22}	11.3	11.0
κ'_{33}	>17.5	15.4

Table 35A-6-017. KTiOPO₄. Electrooptic tensor measured with Fizeau interferometer [92Wan].

r_{ijk}	r_{113}	r_{223}	r_{333}	r_{232}	r_{131}
[pm V ⁻¹]	9.9(4)	13.1(5)	33.1(3)	11.6(4)	8.2(3)

Table 35A-6-018. KTiOPO₄, RbTiOPO₄, KTiOAsO₄, RbTiOAsO₄, CsTiOAsO₄. Nonlinear susceptibilities at $\lambda = 1064$ nm and electrooptic coefficients at $\lambda = 633$ nm [94Che1].

Crystal	Nonlinear susceptibilities at 1.064 μm ^{a)} [pm V ⁻¹]			Electrooptic coefficients at 0.633 μm ^{b)} [pm V ⁻¹]		
	d_{33}	d_{32}	d_{31}	r_{33}	r_{23}	r_{13}
KTiOPO ₄	16.9	4.4	2.5	36.3	15.7	9.5
RbTiOPO ₄	17.1	4.1	3.3	33.0	15.0	10.9
KTiOAsO ₄	16.2	4.2	2.8	37.5	15.4	11.5
RbTiOAsO ₄	15.8	3.8	2.3	40.5	17.5	13.5
CsTiOAsO ₄	18.1	3.4	2.1	38.0	18.5	14.2

^{a)} Uncertainty ± 20 %.^{b)} Uncertainty ± 10 %.

Table 35A-6-019. KTiOPO₄. Raman modes [cm⁻¹] [85Gar]. The underlined frequencies are lines originated from the depolarization effect.

A_1	A_2	B_1	B_2	A_1	A_2	B_1	B_2	A_1	A_2	B_1	B_2
(xx)	(xy)	(xz)	(yz)	(xx)	(xy)	(xz)	(yz)	(xx)	(xy)	(xz)	(yz)
—	—	—	—	—	273	—	—	—	654	<u>653</u>	—
58	<u>58</u>	<u>58</u>	58	280	—	—	—	699	697	696	696
<u>67</u>	67	<u>67</u>	<u>68.5</u>	—	287	298.5	—	—	701	—	—
<u>75</u>	—	<u>75</u>	75	—	—	—	296	—	—	730	—
—	82.5	82	—	299	<u>299</u>	301	299	751	<u>751</u>	—	249
—	86	—	—	—	—	312	310	789	—	786	<u>785.5</u>
89.5	<u>91</u>	91	89	318	<u>318</u>	<u>318</u>	317	—	796	—	—
94	—	—	—	—	329	327	—	—	798	—	—
97	—	<u>97</u>	<u>98</u>	341	342	<u>341</u>	342	—	818	<u>819</u>	<u>817</u>
102	<u>102</u>	101.5	104.5	—	—	—	349	834	—	834	833
114	115	<u>116</u>	116	—	362	363	—	—	966	—	968
121	<u>121</u>	121	122	371	<u>370</u>	372	373	974	977	<u>976.5</u>	—
—	—	<u>124</u>	124	—	382	—	—	—	—	983	—
—	131	—	—	401	400	401	401	—	987	—	—
<u>133</u>	135	<u>134</u>	134	—	413	<u>413</u>	413	990.5	—	993.5	992
—	138	142	—	—	<u>420</u>	<u>420</u>	420	—	1001	—	—
154	152	154	155.5	428	429	429	427	—	—	—	1006
—	—	161	—	—	470	466	466	1009.5	—	—	—
169	166	—	—	476	475	477	476	1025.5	1027.5	—	—
—	—	<u>173</u>	173	486	488	490	488	—	—	1033	1033
177	176	177	—	—	—	503	504	1043	1044	1046	1044
<u>182</u>	—	—	181	—	507	<u>509</u>	—	1100	1097	1097	1095
193	196	194	—	518	<u>518</u>	520	—	1112	1112	—	1115
203	201	203	203	—	539	542	—	—	1125	1129	—
—	209	—	—	547	<u>547</u>	548	548	1137	—	—	1135
214	<u>214</u>	213	215.5	559	557	558	559	1187	—	—	—
—	<u>221</u>	220	224	—	—	561	564	1190	—	—	—
231	235	<u>232.5</u>	232	571	—	—	—	—	—	—	1209
—	—	—	238	594	—	596	593	—	1249	—	—
241	—	240	242.5	600	600	601	599	—	1257	—	—
—	252	<u>253</u>	—	—	—	—	613.5	1293	—	—	—
263	—	—	—	632	632	631	629	1339	—	—	—
<u>268</u>	<u>269</u>	268	269	640	640	640	640	—	—	—	—

Note: The scattering geometries and the types of vibration corresponding to them are indicated; the values of the frequencies are given in reciprocal centimeters.

Table 35A-6-020. KTiOPO₄. Raman and infrared results of the A₁ symmetry [88Kug]. ω_{TO} , ω_{LO} : frequencies [cm⁻¹] of the transverse and longitudinal optic phonon modes. γ , $\Delta\epsilon$: damping and oscillator strength. s: strong; m: medium; w: weak; b: broad; sh: shoulder; db: doublet; v: very. See Fig. 35A-6-062 for the nine frequency regions, I...IX.

Interval	Infrared results				Raman results	
	ω_{TO} [cm ⁻¹]	ω_{LO} [cm ⁻¹]	γ [cm ⁻¹]	$\Delta\epsilon$	Measured frequency [cm ⁻¹]	Intensity [%]
I	78.5	78.7	2.5	0.1	88 sh	1.3
	91	94.2	1.7	1.5	91 w	
	95	96.5	2	0.1	95 sh	
	111	111.2	3	0.06	114 db	
	117.5	117.7	2	0.06	116 db	
	122.5	123.3	1	0.2	121 w	
	129.5	129.6	2	0.03		
	134	135.8	1.5	0.37	132 wb	
II	145	145.5	7	0.1		16.7
	154	154.8	4	0.14	153 m	
	167	167.4	4	0.07	172 m	
	178.7	179.4	6	0.11	178 sh	
	203.7	204.6	3.5	0.2	202 m	
	213	219.2	2	0.4	213 s	
					221 m	
					231 wsh	
III	235	237.6	7	0.5	237 wsh	11.6
	260	261	2.7	0.45		
	268	284.5	4.5	2.5	268 vs	
IV	288	293.2	10	0.2	275 s	8.5
	311	322.5	7	1.4	289 m	
	326	356.4	7	0.4	314 m	
V					323 m	9
					340 s	
					349 wsh	
VI	385	397.2	10	0.7	375 m	5
	400	419.8	8	0.14	400 m	
	428.7	444.9	9	0.15	412 w	
VII	458.7	492.6	15	0.19	420 w	42.3
					464 w	
					475 w	
VIII					508 wsh	1.8
					517 m	
					546 w	
IX	540	542.9	19	0.03	557 w	42.3
					561 wsh	
X	585	586.2	25	0.02	598 w	1.8
	622.5	629.1	30	0.13	632	
	687.5	769	27	0.74	639 mdb	
XI					700 vs	1.8
					724 s	
					794 wb	
XII					834 m	1.8

(continued)

Table 35A-6-020 (continued)

Interval	Infrared results				Raman results	
	ω_{TO} [cm^{-1}]	ω_{LO} [cm^{-1}]	γ [cm^{-1}]	$\Delta\epsilon$	Measured frequency [cm^{-1}]	Intensity [%]
IX	958.7	986.3	12	0.37	968 wsh	3.8
					974 m	
	991.2	1010.5	9	0.03	993 m	
					1008 wsh	
	1023.7	1028.9	8	0.02	1034 w	
	1043.7	1086.4	10	0.09	1043 m	
					1089 wsh	
	1096.2	1119	9	0.01	1099 m	
					1113 wsh	

Table 35A-6-021. KTiOPO₄. Raman and infrared results of B₁ symmetry [88Kug]. See the caption of Table 35A-6-020 for notations.

Interval	Infrared results				Raman results	
	ω_{TO} [cm ⁻¹]	ω_{LO} [cm ⁻¹]	γ [cm ⁻¹]	$\Delta\varepsilon$	Measured frequency [cm ⁻¹]	Intensity [%]
I	74	74.4	4	0.15	74 wsh	1.8
	80	80.4	5	0.18	82 w	
	84.2	85.6	1.5	0.4		
	89.5	90.2	1.5	0.15	88 m	
					92 w	
	103.5	105.9	5	0.53	101 m	
	119	121.3	2	0.37	114 w	
					122 wsh	
	133	133.6	2	0.1	134 m	
	139	139.7	2.5	0.1	141 m	
II	152	152.8	8	0.15	153 w	14.5
	158.7	162.5	4	0.45		
	171	173.8	2	0.21	172 wsh	
					177 s	
					192 m	
					202 m	
	210.5	210.8	2	0.03	213 s	
	221	223.5	4	0.25	221 m	
					231 w	
					238 w	
III	250	250.2	9	0.03	254 msh	17.5
	265	266.8	10	0.25	268 vs	
					275 s	
	289	297	9	1.4	289 m	
					295 wsh	
IV	301	309	9	0.38	313 s	11.3
	318.5	331.3	9	0.55	312 s	
					325 ssh	
V	342	350	15	0.32		6.3
	363.7	398.2	25	0.69	363 msh	
					371 m	
	404	419.1	8	0.08	400 m	
					421 w	
VI	426	438	10	0.05	430 w	3
	467	472.4	12	0.08	463 w	
	486	496.6	13	0.15		
	499	514.5	10	0.02	509 wb	
	556.5	562.7	15	0.05	556 w	
VII					561 w	27.2
	594	598.1	12	0.03	598 w	
	639	651.7	15	0.1	631 w	
					643 w	
					699 vs	
					717 msh	

(continued)

Table 35A-6-021 (continued)

Interval	Infrared results				Raman results	
	ω_{TO} [cm^{-1}]	ω_{LO} [cm^{-1}]	γ [cm^{-1}]	$\Delta\epsilon$	Measured frequency [cm^{-1}]	Intensity [%]
VIII {	781	796	25	0.16	795 vs	} 11.5
	812	821.5	15	0.04	833 wsh	
IX {	975	977.3	15	0.07	984 s	} 6.6
	987	995	17	0.18	994 wsh	

Table 35A-6-022. KTiOPO₄. Raman and infrared results of B₂ symmetry [88Kug]. See the caption of Table 35A-6-020 for notations.

Interval	Infrared results				Raman results	
	ω_{TO} [cm ⁻¹]	ω_{LO} [cm ⁻¹]	γ [cm ⁻¹]	$\Delta\varepsilon$	Measured frequency [cm ⁻¹]	Intensity [%]
I	75 80 90	75.1 80.1 90.1	2 2 1	0.05 0.03 0.1	57 w 74 w	1.9
					88 wsh 92 w	
	92.5	97	2.5	1		
	104.5	109.8	2	0.06		
	116.2	116.6	1.5	0.06	114 w	
	123	124.7	15	0.3	123 w	
	128.5	130	2	0.15	132 w	
II	145 151.2 157.5 175 181 202	146.6 151.9 158.4 175.7 181.7 202.4	15 2 2 4 3 1	0.2 0.06 0.08 0.28 0.06 0.04	153 m	15.2
					172 m	
					178 wsh	
					202 m	
					213 s	
	221.5	223.1	3.5	0.2	221 s	
	231	233.7	4.5	0.23	231 wsh	
III	243 268.7	243.8 272.3	4 5	0.06 0.35	268 vs 275 s	17.8
					290 m	
	291.2	299.1	10	0.6		
IV	331.5	351	8	1.13	314 m 323 s 334 wsh	11.2
V	380 393.7	388.3 410.3	15 14	0.7 0.4	369 m 381 wsh 401 m	5.4
	416.2	472.4	25	0.22	420 w 429 w	
VI	499 553.7	500.8 561.2	20 12	0.01 0.08	462 wb 547 w 556 w 561 wsh	1
VII	596.2 631.2	598.7 642.3	9 20	0.03 0.13	598 w 632 mdb 639 mdb	45.5
	673.7 698.7	674 737.6	3 20	0.004 0.28	700 vs 727 m	

(continued)

Table 35A-6-022 (continued)

Interval	Infrared results				Raman results	
	ω_{TO} [cm ⁻¹]	ω_{LO} [cm ⁻¹]	γ [cm ⁻¹]	$\Delta\varepsilon$	Measured frequency [cm ⁻¹]	Intensity [%]
VIII	826.2	827.8	20	0.01	793 wb	0.5
	863.7	864	25	0.002	834 w	
IX	970	982	8	0.15	968 vw	1.5
					994 w	
	1019	1028.7	8	0.2		
	1035	1098.4	16	0.11	1044 w	
	1119	1136.2	10	0.01	1110 w	
					1129 w	

Table 35A-6-023. KTiOPO₄, KTiOAsO₄, RbTiOPO₄. Internal Raman mode assignments [91Wat]. The internal and representative features assigned to vibrational modes of the (As, P)O₄ tetrahedron and TiO₆ octahedron are listed. Frequency [cm⁻¹] spread of features in different geometries is shown in parentheses.

Group	Mode	Interval	KTiOAsO ₄ frequency [cm ⁻¹]	KTiOPO ₄ frequency [cm ⁻¹]	KTiOPO ₄ – KTiOAsO ₄ shift [%]	RbTiOPO ₄ frequency [cm ⁻¹]	Geometry
TiO ₆	ν_1	VIIb	669.8	692.8	3.4	687.2	$A_1(zz)$
			673.0	698.8	3.8	693.4	$A_1(xx)$
			(3.2)	(6.0)			
	ν_2	VIIb	703.6	728.2	3.5	723.4	$A_1(yy)$
			722.4	754.2	4.4	749.2	$A_1(xx)$
			(18.8)	(26.0)			
	ν_3	VIII	747.4	795.0	6.4	793.2	B_1
			776.8	834.0	7.4	834.2	$A_1(yy)$
			781.8	818.6	4.7	816.8	A_2
			(34.4)	(39.0)			
	ν_4	VIIa (VI, KTP)	491.2	517.2	5.3	519.4	$A_1(xx)$
			513.4	546.6	6.5	550.2	$A_1(xx)$
	ν_5	III	(22.2)	(29.4)			
			234.0	268.0	14.5	270.8	$A_1(zz)$
	ν_6	II	250.0	267.8	7.1	265.0	B_2
			188.4	201.6	7.0	203.6	B_2
			205.0	220.8	7.7	228.0	B_2
(As, P)O ₄	ν_1	IX	(16.6)	(19.2)			
			810.2	980.4	21.0	969.4	B_1
	ν_2	V	342.8	400.6	16.9	395.4	$A_1(xx)$
			370.8	428.2	15.5	421.8	$A_1(xx)$
	ν_3	IX	871	1046	16.7	1036	$A_1(zz)$ av.
	ν_4	VIIa	509.8	631.4	23.9	622.4	$A_1(xx)$
			531.8	646.6	21.6	639.0	B_1

Table 35A-6-024. KTiOPO₄. Electrical data of crystals doped with various metals [91McG]. Crystal growth: high temperature solution method.

Dopant	Concentration in crystal [ppm]	Conductivity [10 ² Ω ⁻¹ m ⁻¹]	Growth tempera- ture range [°C]
Cr	50	8.0 · 10 ⁻⁷	967–944
Cr	100	5.0 · 10 ⁻⁷	963–931
Cr	70	3.0 · 10 ⁻⁹	962–935
Ga	50	2.0 · 10 ⁻⁶	954–936
Ga	50	1.0 · 10 ⁻⁶	956–935
Ga	30	1.0 · 10 ⁻⁶	953–930
Ga	600	1.0 · 10 ⁻⁷	943–924
Ga	1000	3.0 · 10 ⁻⁹	946–898
Ga	1300	2.5 · 10 ⁻⁹	938–893
Ga	1000	2.0 · 10 ⁻⁹	968–922
Al	20	3.0 · 10 ⁻⁶	961–940
Al	60	1.1 · 10 ⁻⁶	957–931
Al	70	1.1 · 10 ⁻⁶	946–915
Al	175	6.0 · 10 ⁻⁷	957–937
Al	100	1.3 · 10 ⁻⁷	943–921
Al	440	2.3 · 10 ⁻⁹	935–900
Al	105	1.2 · 10 ⁻⁹	957–919
Al	250	1.0 · 10 ⁻⁸	966–946
Mg	30	–	956–930
Mg	30	–	959–925
Mg	150	3.0 · 10 ⁻⁷	962–936
Li	< 10	1.5 · 10 ⁻⁶	957–909
V	20	5.0 · 10 ⁻⁷	963–939

Table 35A-6-025. KTiOPO₄, RbTiOPO₄. Luminescence data at 4.2 K [90Bla].

	KTiOPO ₄	RbTiOPO ₄
Maximum of emission band [nm]	390	410
Maximum of excitation band [nm]	340	320
Maximum of emission band [cm ⁻¹]	25.200	23.800
Maximum of excitation band [cm ⁻¹]	29.400	31.250
Stokes shift [cm ⁻¹]	4.200	7.450

Table 35A-6-026. KTiOPO₄:Fe³⁺. Fe³⁺ spin Hamiltonian parameters of the four centers designated as ST1, ST2, ST3 and ST4 [91Gai].

	ST1	ST3	ST2	ST4
<i>ij</i>	Matrix components g_{ij}			
<i>xx</i>	1.9997	1.9995	2.0027	2.0027
<i>yy</i>	2.0037	2.0055	2.0026	2.0045
<i>zz</i>	2.0038	2.0045	2.0056	2.0048
<i>xy</i>	-0.0015	0.0050	0.0009	0.0037
<i>xz</i>	0.0003	-0.0019	-0.0011	0.0006
<i>yz</i>	-0.0001	0.0000	-0.0008	0.0001
<i>m</i>	Normalized second-order constants B_2^m [10^{-2} m ⁻¹]			
0	261.5	278.6	167.5	200.3
1	314.1	117.0	-647.6	-621.0
-1	-334.5	-692.3	142.3	176.7
2	264.0	411.7	-356.2	-338.4
-2	-126.6	-47.3	-139.3	-220.0
<i>m</i>	Normalized fourth-order constants $60 B_4^m$ [10^{-2} m ⁻¹]			
0	32.0	28.0	21.7	24.4
1	2.4	3.1	7.1	7.3
-1	10.0	9.8	3.2	3.8
2	-68.0	-50.2	47.1	56.9
-2	-12.3	-4.9	17.2	18.7
3	2.2	-1.8	-18.5	-11.5
-3	23.1	22.7	6.8	-2.9
4	-28.3	-19.2	-12.0	-18.0
-4	-3.0	-2.9	-12.0	-16.3

$$H = \sum_{ij} \beta B_i g_{ij} S_j + \sum_{m=-2}^2 B_2^m O_2^m + \sum_{m=-4}^4 B_4^m O_4^m.$$

Table 35A-6-027. KTiOPO₄:VO²⁺. Spin Hamiltonian parameters for VO²⁺ in Ti(1) sites [89Vas]. θ and φ are the angles to the *b* axis and of the projection onto the *ac*-plane to the *a* axis, respectively.

i	g_{ii}	θ	φ	A_{ii} [$\cdot 10^{-2}$ m ⁻¹]	θ	φ
<i>x</i>	1.975(5)	77.5°	87.6°	60.8(2)	51.0°	137.7°
<i>y</i>	1.981(3)	43.3°	163.7°	50.6(2)	57.5°	68.2°
<i>z</i>	1.937(5)	46.4°	10.1°	175.4(3)	49.3°	19.3°

Table 35A-6-028. KTiOPO₄:V⁴⁺. ESR spin Hamiltonian parameters [94Liu]. Spin Hamiltonian: $H = \beta S \cdot g \cdot B + S \cdot A \cdot I$. Hyperfine constants are expressed in units of 10^{-2} m^{-1} . The direction cosines of the principal axes are expressed relative to the a , b and c axes of the orthorhombic host. The estimated error in g is ± 0.001 and in the hyperfine constants $\pm 10^{-2} \text{ m}^{-1}$.

Species	Principal values and axes		Symmetry
	g	A	
V ⁴⁺ ₍₁₎	$g_{\parallel} = 1.933$	$A = 167.4$	Axial
	$g_{\perp} = 1.959$	$B = 54.0$	
	$\hat{n} = (-0.6993, 0.1290, -0.7096)$		
	$g_x = 1.959$	$A_x = 54.0$	Non-axial
	$g_y = 1.958$	$A_y = 54.0$	
	$g_z = 1.935$	$A_z = 167.5$	
V ⁴⁺ ₍₂₎	$g_{\parallel} = 1.939$	$A = 168.5$	Axial
	$g_{\perp} = 1.953$	$B = 54.5$	
	$\hat{n} = (-0.1651, 0.6876, -0.7071)$		
	$g_x = 1.958$	$A_x = 54.1$	Non-axial
	$g_y = 1.949$	$A_y = 55.5$	
	$g_z = 1.938$	$A_z = 168.3$	

Table 35A-6-029. KTiOPO₄:V⁴⁺. Spin Hamiltonian parameters [92Han]. Principal values of the g tensor and direction cosines of its principal axes (x' , y' , z') with respect to the coordinate system (x , y , z) for two kinds of site. The direction cosines of other three sets of four physically equivalent but magnetically non-equivalent sites are obtained through the relations: \bar{l} , m , n ; l , \bar{m} , \bar{n} for each kind of site. Principal values of A and direction cosines of its principal axes (x'' , y'' , z'') with respect to the coordinate system (x' , y' , z') for two kinds of sites. Principal values are expressed in GHz. $H = \mu_B S \cdot g \cdot B + S \cdot A \cdot I$. $S = 1/2$, $I = 7/2$.

Sites	Principal values	Direction cosines			
		x	y	z	
I	$g_{x'}=1.9825$	l	0.1969	-0.6816	0.7047
	$g_{y'}=1.9659$	m	0.9573	0.2887	0.0119
	$g_{z'}=1.9342$	n	-0.2116	0.6723	0.7094
II	$g_{x'}=1.9730$	l	0.7975	-0.0542	-0.6009
	$g_{y'}=1.9596$	m	0.2110	0.9581	0.1936
	$g_{z'}=1.9369$	n	0.5652	-0.2812	0.7755

Sites	Principal values	Direction cosines		
		x	y	z
I	$A_{x''}=0.1809$	-0.9453	0.3204	-0.0615
	$A_{y''}=0.1594$	-0.3222	-0.8876	0.3293
	$A_{z''}=0.4994$	0.0509	0.3311	0.9422
II	$A_{x''}=0.1828$	-0.9615	-0.1745	0.2125
	$A_{y''}=0.1610$	0.2486	-0.8817	0.4010
	$A_{z''}=0.5044$	0.1174	0.4384	0.8911

Table 35A-6-030. KTiOPO₄:V⁴⁺. EPR spin Hamiltonian parameters for V⁴⁺ [92Han]. x, y, z : crystal coordinates; x', y', z' : principal axes for g ; x'', y'', z'' : principal axes for A .

Sites	Principal values	Direction cosines		
		x	y	z
I	$g_{x'} = 1.9825$	l	0.1969	−0.6816
	$g_{y'} = 1.9659$	m	0.9573	0.2887
	$g_{z'} = 1.9342$	n	−0.2116	0.6723
II	$g_{x'} = 1.9730$	l	0.7975	−0.0542
	$g_{y'} = 1.9596$	m	0.2110	0.9581
	$g_{z'} = 1.9369$	n	0.5652	−0.2812

Sites	Principal values	Direction cosines		
		x	y	z
I	$A_{x''} = 0.1809$	−0.9453	0.3204	−0.0615
	$A_{y''} = 0.1594$	−0.3222	−0.8876	0.3293
	$A_{z''} = 0.4994$	0.0509	0.3311	0.9422
II	$A_{x''} = 0.1828$	−0.9615	−0.1745	0.2125
	$A_{y''} = 0.1610$	0.2486	−0.8817	0.4010
	$A_{z''} = 0.5044$	0.1174	0.4384	0.8911

Table 35A-6-031. KTiOPO₄:Cr³⁺. Cr³⁺ ($S = 3/2$) spin Hamiltonian parameters of the two sites belonging to the centers A and B, respectively, in the X, Y, Z crystallographic axis system [95Ahn]. Spin-Hamiltonian: $H = \sum \mu B_i \cdot g_{ij} \cdot S_j + \sum B_2^m O_2^m$.

	A	B
ij	Matrix components g_{ij}	
XX	1.96379(15)	1.97261(16)
YY	1.97552(18)	1.96749(17)
ZZ	1.97143(19)	1.97261(17)
XY	0.00063(19)	−0.00066(17)
XZ	−0.00068(17)	−0.00156(18)
YZ	−0.00093(23)	0.00073(17)

Second-order FS parameters		
m	$B_2^m [10^2 \text{ m}^{-1}]$	
0	−0.11660(3)	−0.08577(2)
1	0.00585(11)	0.21558(9)
−1	−0.13399(11)	−0.08525(9)
2	0.21050(4)	−0.17181(3)
−2	−0.05781(5)	0.07148(4)

Table 35A-6-032. KTiOPO₄:W⁵⁺. Spin Hamiltonian parameters for W⁵⁺ [95Ang]. *l, m, n*: direction cosines relative to the crystal (*a, b, c*) system. Sample: crystal grown from molten tungstate solutions.

Principal values			Principal axes				
			l	m	n	θ [deg]	ϕ [deg]
W1	g_x	1.6037(6)	0.980	−0.147	0.133	82.4(2)	351.4(4)
	g_y	1.5406(8)	0.185	0.917	−0.352	110.6(4)	78.6(4)
	g_z	1.4634(8)	−0.071	0.370	0.926	22.1(4)	100.8(6)
	$ A_x $	$77(3) \cdot 10^2 \text{ m}^{-1}$	0.781	−0.282	0.558	56(2)	340(10)
	$ A_y $	$92(2) \cdot 10^2 \text{ m}^{-1}$	0.285	0.955	0.083	85(4)	73(6)
	$ A_z $	$136(3) \cdot 10^2 \text{ m}^{-1}$	−0.556	0.094	0.826	34(2)	170(5)
			l	m	n	θ [deg]	ϕ [deg]
W2	g_x	1.6064(8)	−0.323	−0.941	0.106	83.9(4)	251.1(8)
	g_y	1.5636(8)	0.947	−0.320	0.041	87.7(8)	341.3(8)
	g_z	1.5046(6)	−0.005	0.113	0.994	6.5(4)	92(6)
	$ A_x $	$82(4) \cdot 10^2 \text{ m}^{-1}$	−0.257	−0.776	0.576	55(2)	252(15)
	$ A_y $	$97(3) \cdot 10^2 \text{ m}^{-1}$	0.943	−0.332	−0.027	92(7)	341(7)
	$ A_z $	$151(3) \cdot 10^2 \text{ m}^{-1}$	0.212	0.536	0.817	35(2)	68(6)

Table 35A-6-033. KTiOPO₄:Mo⁵⁺. Spin Hamiltonian parameters at 77K [92Gei].

$ A_x = 64.0(5) \cdot 10^{-2} \text{ m}^{-1}$	$g_x = 1.905(1)$
$ A_y = 76.0(7) \cdot 10^{-2} \text{ m}^{-1}$	$g_y = 1.857(1)$
$ A_z = 86(1) \cdot 10^{-2} \text{ m}^{-1}$	$g_z = 1.837(1)$

Table 35A-6-034. KTiOPO₄:Rh³⁺. ESR spin Hamiltonian parameters for centers Rh1 and Rh2 observed at 90 K [94Bra]. The HF parameters are given in units of 10⁻² m⁻¹. The *g* and *A* matrices are expressed in both the (*a*, *b*, *c*) crystal axes system and diagonal form. Labelling of the principal *g* values has been made by decreasing magnitude and realizing that the diagonal *g* matrix is nearly axial. Principal axes of *A* are labelled according to the closest principal *g* axis. The orientations of the principal axes are expressed both with direction cosines, [*l*, *m*, *n*], and polar coordinates, (*θ*, *φ*), referred to the (*a*, *b*, *c*) system. The *g* and *A* matrices are given for one Rh1 center and one Rh2 center. The symmetry elements of the crystal lattice provide the matrices for the three other equivalent centers in each case.

		a	b			c	
Rh1	g matrix	a	2.3103 (3)				
		b	0.0162 (4)	2.5681 (3)			
		c	0.3054 (3)	−0.0158 (4)	2.2295 (3)		
	A matrix	a	30.1 (3)				
		b	1.0 (4)	33.3 (3)			
		c	2.8 (3)	0.3 (4)	28.4 (3)		
Rh2	g matrix	a	2.5830 (3)				
		b	−0.0497 (4)	2.2577 (3)			
		c	−0.0638 (4)	−0.2865 (3)	2.2627 (3)		
	A matrix	a	32.9 (3)				
		b	−0.9 (4)	27.5 (3)			
		c	−0.2 (4)	−2.2 (3)	27.4 (3)		
		Principal values	Principal axes				
			l	m	n	θ [deg]	ϕ [deg]
Rh1	g_x	2.5783 (7)	0.744	0.183	0.643	50.0 (5)	14 (3)
	g_y	2.5686 (4)	0.114	−0.982	0.148	81 (2)	277 (2)
	g_z	1.9610 (6)	0.659	−0.037	−0.751	138.7 (1)	356.8 (1)
	A_x	31.6 (8)	0.676	−0.497	0.543	57 (5)	324 (9)
	A_y	33.9 (6)	−0.425	−0.866	−0.264	105 (9)	244 (9)
	A_z	26.3 (5)	0.602	−0.052	−0.797	143 (4)	355 (7)
Rh2	g_x	2.5955 (4)	0.971	0.055	−0.234	103.5 (3)	3.3 (4)
	g_y	2.5446 (7)	0.203	−0.709	0.675	47.6 (2)	286.0 (6)
	g_z	1.9633 (7)	−0.128	−0.703	−0.700	134.4 (1)	259.6 (1)
	A_x	33.1 (4)	0.984	−0.172	0.032	88 (8)	350 (7)
	A_y	29.6 (2)	−0.144	−0.689	0.710	45 (11)	258 (9)
	A_z	25.2 (2)	−0.100	−0.704	−0.704	135 (4)	262 (15)

Table 35A-6-035. KTiOPO₄. KTP waveguide characteristics [87Bie2]. Waveguides are fabricated using molten nitrate salts. Temp.: temperature of the salt. Time: immersion time. d : diffusion depth. Δn : increase in refractive index.

Ion	Surface type	T [°C]	t [h]	No. of modes	Mode type	d [μm]	Δn
Rb	x	450	3.3	0	TE		
				1	TM	1.3	0.02
Rb	$z(+)$	350	4	3	TE	4.0	0.019
				3	TM	4.0	0.018
Rb	$z(-)$	350	4	3	TE	6.5	0.008
				2	TM	6.5	0.008
Cs	z	450	4	11	TE	13	0.028
				8	TM	13	0.019
Tl	z	335	4	4	TE	1.6	0.23
				4	TM	1.6	0.18