

Table 35A-21-001. RbTiOAsO₄, KTiOPO₄, RbTiOPO₄, KTiOAsO₄, KTiO(P_{0.58}As_{0.42})O₄, (Rb_{0.465}K_{0.535})TiOPO₄. Atomic coordinates, temperature parameters (a) and bond lengths (b) [92Tho]. U_{iso} : isotropic temperature parameter. *) Works in [86ElB].

(a)

	x	y	z	$U_{\text{iso}} [\text{\AA}^2]$
KTiO(P _{0.58} As _{0.42})O ₄				
Ti(1)	0.37381(4)	0.5019(1)	0.00036(7)	0.0069(1)
Ti(2)	0.24689(5)	0.26967(8)	0.74914(7)	0.0070(1)
(As,P)(1)	0.49832(4)	0.33205(7)	0.74080(7)	0.0063(1)
(As,P)(2)	0.18015(4)	0.50396(9)	0.48799(7)	0.0083(1)
K(1)	0.37724(7)	0.7800(1)	0.6868(1)	0.0224(3)
K(2)	0.10667(7)	0.6991(1)	0.9321(1)	0.0230(3)
O(1)	0.4872(2)	0.4898(5)	0.8525(2)	0.0125(8)
O(2)	0.5085(2)	0.4647(5)	0.6130(3)	0.0124(8)
O(3)	0.3975(2)	0.1912(4)	0.7200(2)	0.0120(8)
O(4)	0.5956(2)	0.1852(4)	0.7598(2)	0.0133(8)
OT(1)	0.2232(2)	0.9621(4)	0.3578(2)	0.0095(7)
OT(2)	0.2209(2)	0.0468(5)	0.6096(2)	0.0096(7)
O(5)	0.1103(2)	0.3081(4)	0.4569(2)	0.0111(7)
O(6)	0.1094(2)	0.6972(4)	0.5136(2)	0.0128(7)
O(7)	0.2562(2)	0.5406(5)	0.3698(2)	0.0127(8)
O(8)	0.2556(2)	0.4615(5)	0.6036(2)	0.0135(8)
(Rb _{0.465} K _{0.535})TiOPO ₄				
Ti(1)	0.37312(4)	0.49367(9)	0.00154(7)	0.0051(1)
Ti(2)	0.24924(5)	0.26404(9)	0.74734(7)	0.0049(1)
P(1)	0.49988(7)	0.3344(1)	0.7410(1)	0.0053(2)
P(2)	0.18169(6)	0.4965(1)	0.4882(9)	0.0059(2)
(K,Rb)(1)	0.37876(6)	0.7770(1)	0.68696(8)	0.0194(2)
(K,Rb)(2)	0.10318(3)	0.68387(7)	0.92873(6)	0.0173(1)
O(1)	0.4857(2)	0.4786(4)	0.8538(2)	0.0092(7)
O(2)	0.5118(2)	0.4685(4)	0.6195(2)	0.0083(8)
O(3)	0.4033(2)	0.1965(4)	0.7202(2)	0.0072(7)
O(4)	0.5965(2)	0.1964(4)	0.7578(2)	0.0094(7)
OT(1)	0.2215(2)	0.9582(4)	0.3563(2)	0.0079(7)
OT(2)	0.2242(2)	0.0352(4)	0.6092(2)	0.0068(7)
O(5)	0.1144(2)	0.3042(4)	0.4599(2)	0.0086(8)
O(6)	0.1125(2)	0.6844(4)	0.5144(2)	0.0094(7)
O(7)	0.2506(2)	0.5365(4)	0.3709(2)	0.0090(7)
O(8)	0.2548(2)	0.4551(4)	0.5992(2)	0.0092(7)

(continued)

Table 35A-21-001a (continued)

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [Å ²]
RbTiOPO ₄				
Ti(1)	0.37284(6)	0.4998(1)	0.00081(9)	0.0066(3)
Ti(2)	0.24836(7)	0.2678(1)	0.74858(9)	0.0067(3)
P(1)	0.4997(1)	0.3332(2)	0.7422(1)	0.0070(4)
P(2)	0.18035(9)	0.5014(2)	0.4884(1)	0.0079(4)
Rb(1)	0.38504(4)	0.78347(8)	0.67465(7)	0.0205(2)
Rb(2)	0.10537(4)	0.69184(9)	0.92598(8)	0.0176(2)
O(1)	0.4862(3)	0.4786(7)	0.8535(4)	0.008(1)
O(2)	0.5141(3)	0.4604(7)	0.6199(3)	0.009(1)
O(3)	0.4024(2)	0.2026(5)	0.7207(3)	0.009(1)
O(4)	0.5949(3)	0.1943(6)	0.7616(4)	0.011(1)
OT(1)	0.2218(3)	0.9607(6)	0.3564(4)	0.008(1)
OT(2)	0.2226(3)	0.0437(7)	0.6097(3)	0.009(1)
O(5)	0.1141(3)	0.3109(6)	0.4583(3)	0.009(1)
O(6)	0.1128(3)	0.6894(6)	0.5174(4)	0.012(1)
O(7)	0.2505(3)	0.5423(6)	0.3729(3)	0.009(1)
O(8)	0.2522(3)	0.4576(6)	0.6010(4)	0.011(1)
RbTiOAsO ₄				
Ti(1)	0.37382(8)	0.5046(2)	0.0015(1)	
Ti(2)	0.2488(1)	0.2693(3)	0.7514(1)	
As(1)	0.49960(6)	0.32823(9)	0.7444(1)	
As(2)	0.17996(5)	0.5049(1)	0.4903(1)	
Rb(1)	0.38303(6)	0.7825(1)	0.6729(7)	
Rb(2)	0.10900(5)	0.6938(1)	0.9261(1)	
O(1)	0.4875(4)	0.4889(9)	0.8614(4)	
O(2)	0.9892(4)	0.962(1)	0.1107(4)	
O(3)	0.3940(4)	0.1878(7)	0.7228(4)	
O(4)	0.9000(3)	0.6775(7)	0.2469(4)	
OT(1)	0.2169(4)	0.0544(5)	0.6103(4)	
OT(2)	0.7188(4)	0.5489(9)	0.3620(4)	
O(5)	0.1093(4)	0.3032(8)	0.4527(4)	
O(6)	0.6073(4)	0.7961(8)	0.5222(4)	
O(7)	0.2576(4)	0.5445(9)	0.3675(4)	
O(8)	0.7576(4)	0.0408(9)	0.6098(4)	

(b)

	KTP	RKTP	RTP	KTAP	KTA	RTA
Ti(1)–O6 octahedron						
Ti(1)–O(1)	2.150(3)	2.138(2)	2.146(4)	2.160(2)	2.138(15)	2.135(5)
Ti(1)–O(2)	1.958(3)	1.956(3)	1.950(4)	1.955(3)	1.947(16)	1.949(5)
Ti(1)–OT(1)	1.981(3)	1.978(2)	1.973(4)	1.993(2)	1.957(16)	1.973(5)
Ti(1)–OT(2)	1.716(3)	1.717(2)	1.714(4)	1.719(2)	1.735(16)	1.717(5)
Ti(1)–O(5)	2.043(3)	2.052(3)	2.076(4)	2.048(3)	2.002(18)	2.075(5)
Ti(1)–O(6)	1.987(3)	2.003(3)	2.032(4)	1.991(3)	2.004(19)	2.037(5)

(continued)

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Table 35A-21-001b (continued)

	KTP	RKTP	RTP	KTAP	KTA	RTA
Ti(2)–O6 octahedron						
Ti(2)–O(3)	2.044(3)	2.056(3)	2.063(3)	2.040(3)	2.024(14)	2.026(5)
Ti(2)–O(4)	1.981(3)	1.989(3)	2.011(4)	1.987(2)	1.989(14)	2.011(4)
Ti(2)–OT(1)	1.733(3)	1.742(2)	1.737(4)	1.747(3)	1.770(19)	1.755(5)
Ti(2)–OT(2)	2.092(3)	2.102(2)	2.094(4)	2.103(3)	2.097(19)	2.133(4)
Ti(2)–O(7)	1.964(3)	1.963(3)	1.967(4)	1.967(3)	1.941(19)	1.962(6)
Ti(2)–O(8)	1.990(3)	1.994(2)	1.989(4)	1.994(3)	1.983(18)	1.993(5)
As,P(1)–O4 tetrahedron						
P(1)–O(1)	1.518(2)	1.523(2)	1.518(4)	1.579(3)	1.630(19)	1.663(5)
P(1)–O(2)	1.548(2)	1.559(2)	1.544(4)	1.620(3)	1.720(18)	1.699(5)
P(1)–O(3)	1.544(3)	1.547(3)	1.538(3)	1.609(3)	1.714(14)	1.701(5)
P(1)–O(4)	1.541(3)	1.542(3)	1.543(4)	1.593(3)	1.656(14)	1.684(6)
As,P(2)–O4 tetrahedron						
P(2)–O(5)	1.535(3)	1.541(3)	1.538(4)	1.594(3)	1.694(16)	1.691(5)
P(2)–O(6)	1.528(3)	1.528(3)	1.533(4)	1.575(3)	1.635(18)	1.678(5)
P(2)–O(7)	1.548(3)	1.551(2)	1.545(4)	1.620(2)	1.704(16)	1.698(5)
P(2)–O(8)	1.537(2)	1.531(3)	1.538(4)	1.600(2)	1.679(18)	1.676(5)
M(1)–O cage						
M(1)–O(1)	2.894(3)	2.952(3)	3.036(4)	2.951(3)	2.981*	3.145(5)
M(1)–O(2)	2.738(3)	2.720(3)	2.747(4)	2.773(3)	2.771*	2.808(6)
M(1)–O(3)	2.712(3)	2.740(3)	2.774(3)	2.701(3)	2.653*	2.765(5)
M(1)–OT(1)	2.996(3)	3.017(3)	3.162(4)	3.046(3)	3.098*	3.297(5)
M(1)–OT(2)	2.723(3)	2.724(3)	2.786(4)	2.788(3)	2.872*	2.935(5)
M(1)–O(5)	2.871(3)	2.899(3)	3.002(4)	2.898(2)	2.895*	3.017(4)
M(1)–O(6)			3.395(4)			3.390(5)
M(1)–O(7)	3.057(4)	3.062(3)	3.210(4)	3.109(3)	3.154*	3.307(5)
M(1)–O(8)	2.755(3)	2.778(3)	2.838(4)	2.745(3)	2.717*	2.811(6)
M(2)–O cage						
M(2)–O(1)	2.677(3)	2.765(3)	2.749(4)	2.681(3)	2.691*	2.753(6)
M(2)–O(2)	2.982(3)	3.105(3)	3.105(3)	2.988(3)	3.009*	3.109(5)
M(2)–O(3)	3.045(3)	3.091(3)	3.117(4)	3.079(2)	3.128*	3.196(4)
M(2)–O(4)	3.117(4)	3.045(3)	3.052(4)	3.100(3)	3.067*	3.030(5)
M(2)–OT(1)	2.765(3)	2.796(3)	2.797(4)	2.802(3)	2.861*	2.885(5)
M(2)–OT(2)	3.056(2)	3.088(3)	3.110(4)	3.093(3)	3.150*	3.183(5)
M(2)–O(5)	2.806(3)	2.829(3)	2.870(4)	2.826(3)	2.848*	2.910(5)
M(2)–O(7)	2.917(3)	3.014(3)	2.998(4)	2.915(3)	2.908*	3.002(6)
M(2)–O(8)	3.047(3)	3.109(3)	3.132(4)	3.072(3)	3.117*	3.192(5)

Note: KTP: KTiOPO₄RKTP: (K_{0.535}Rb_{0.456})TiOPO₄RTP: RbTiOPO₄KTAP: KTiO(P_{0.54}As_{0.46})O₄KTA: KTiOAsO₄RTA: RbTiOAsO₄

Table 35A-21-002. RbTiOAsO₄. Refractive indices at 20 °C [93Han]. Parameter: λ .

λ [Å]	n_x	n_y	n_z
6562.8	1.8267	1.8352	1.9142
5875.6	1.8364	1.8456	1.9279
5460.7	1.8444	1.8543	1.9397
4861.3	1.8405	1.8720	1.9643
5320.0	1.8476	1.8578	1.9444
10640.0	1.8041	1.8114	1.8846