

Table 35A-9-001. RbTiOPO₄. Atomic coordinates and anisotropic temperature parameters [93Kad]. $T = 293\text{K}$. For definition of U_{ij} , see Eq. (d) in Introduction.

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti(1)	0.37276(8)	0.4997(2)	0.0	0.0175(4)	0.0151(6)	0.0191(6)	0.0002(4)	0.0001(4)	0.0011(5)
Ti(2)	0.24834(9)	0.2682(2)	0.2518(3)	0.0178(4)	0.0154(6)	0.0182(6)	-0.0004(3)	0.0006(4)	-0.0001(6)
P(1)	0.4998(1)	0.3335(3)	0.2583(3)	0.0173(6)	0.0142(8)	0.0199(8)	-0.0001(5)	-0.0007(5)	0.0011(9)
P(2)	0.1802(1)	0.5017(4)	0.5120(3)	0.0186(6)	0.0157(9)	0.0187(9)	-0.0001(5)	0.0005(6)	-0.0012(7)
Rb(1)	0.38488(6)	0.7836(2)	0.3258(2)	0.0310(4)	0.0187(4)	0.0404(6)	0.0040(2)	0.0056(4)	0.0014(5)
Rb(2)	0.10548(5)	0.6919(2)	0.0745(2)	0.0232(3)	0.0247(4)	0.0359(5)	0.0044(2)	0.0006(3)	0.0013(4)
O(1)	0.4862(4)	0.479(1)	0.1459(8)	0.021(2)	0.021(3)	0.021(3)	-0.004(2)	-0.005(2)	0.009(3)
O(2)	0.5140(5)	0.462(1)	0.3806(8)	0.022(2)	0.023(3)	0.023(3)	0.002(2)	-0.002(2)	-0.002(3)
O(3)	0.4022(4)	0.205(1)	0.2807(8)	0.017(2)	0.018(3)	0.029(3)	0.000(2)	0.000(2)	-0.000(3)
O(4)	0.5939(4)	0.193(1)	0.2375(8)	0.015(2)	0.019(3)	0.029(3)	0.001(1)	0.002(2)	-0.003(3)
O(5)	0.1137(4)	0.312(1)	0.5423(7)	0.028(2)	0.017(3)	0.019(3)	-0.002(2)	0.003(2)	0.002(2)
O(6)	0.1131(4)	0.690(1)	0.4842(9)	0.025(2)	0.018(3)	0.027(4)	0.002(2)	-0.003(2)	0.002(3)
O(7)	0.2507(4)	0.542(1)	0.6266(7)	0.021(2)	0.021(3)	0.020(3)	0.001(2)	-0.002(2)	-0.002(2)
O(8)	0.2522(5)	0.459(1)	0.4005(8)	0.025(2)	0.020(3)	0.024(3)	-0.005(2)	0.003(2)	-0.000(3)
O(9)	0.2777(4)	0.462(1)	0.1440(7)	0.022(2)	0.021(3)	0.017(3)	0.004(2)	0.002(2)	0.003(2)
O(10)	0.2227(4)	0.043(1)	0.3911(7)	0.023(2)	0.018(3)	0.022(3)	0.001(2)	0.001(2)	0.001(2)

Table 35A-9-002. RbTiOPO₄. $d_{i\lambda}$, $e_{i\lambda}$, k_{ij} , κ_{ij} , $s_{\lambda\mu}^E$, $c_{\lambda\mu}^E$ [90Sil].

d_{31}	4.17 [10 ⁻¹² C N ⁻¹]	k_{31}	0.122	s_{11}^E	70.926 [10 ⁻¹⁰ m ² N ⁻¹]
d_{32}	3.57	k_{32}	0.112	s_{22}^E	61.95
d_{33}	11.34	k_{33}	0.306	s_{33}^E	78.67
d_{15}	10.09	k_t	0.201	s_{44}^E	134
d_{24}	4.94	k_{15}	0.08	s_{55}^E	184.16
e_{33}	1.08 [C m ⁻²]	k_{24}	0.118	c_{33}^E	17.51 [10 ¹⁰ N m ⁻²]
e_{15}	0.18	κ_{11}	11	c_{44}^E	7.46
e_{24}	0.37	κ_{22}	15	c_{55}^E	5.49
		κ_{33}	18.54–17.9		

Table 35A-9-003. RbTiOPO₄. n_x , n_y , n_z as functions of λ [90Wan]. $T = 293\text{ K}$.

λ [Å]	n_x	n_y	n_z
7065.3	1.7793	1.7882	1.8745
6678.1	1.7829	1.7921	1.8798
5892.9	1.7928	1.8028	1.8945
5875.6	1.7930	1.8031	1.8949
5460.74	1.8003	1.8110	1.9058
5015.7	1.8106	1.8226	1.9218
4471.5	1.8289	1.8432	1.9511
4358.35	1.8340	1.8490	1.9592

Table 35A-9-004. RbTiOPO_4 . Raman shifts of A_1 , A_2 , B_1 , B_2 modes [cm^{-1}] [92Wan]. s: strong; w: weak; m: medium; v: very.

A_1 (TO)	A_1 (LO)	A_2	B_1	B_2
50(w)	50(w)			
61(w)	62(w)	58(w)	56(w)	58(w)
73(w)	73(m)			77(vw)
104(m)	104(m)	105(m)	104(m)	104(m)
111(vw)		120(w)		119(w)
		137(w)		138(w)
142(w)	143(w)		141(w)	
159(m)	160(m)			
163(m)		164(m)	165(s)	202(s)
211(vs)	213(s)			210(m)
		228(s)	226(vs)	225(s)
269(vs)	270(w)	265(vs)	266(vs)	268(vs)
289(s)	289(m)		286(m)	287(m)
299(m)	298(w)			
313(w)	315(w)	313(s)	312(s)	310(s)
		328(vs)	328(vs)	330(s)
367(s)	368(vs)	370(m)	366(m)	366(m)
393(m)	394(s)	395(w)	396(w)	393(w)
417(m)	417(s)	416(m)	415(m)	418(m)
423(m)				
463(w)	476(s)	463(w)	463(w)	
494(w)	494(w)			
517(s)	517(s)			
549(s)	548(s)			
	560(w)			
584(w)	585(w)			
629(w)		631(m)	632(s)	632(m)
689(vs)	689(s)			
693(w)	693(w)	695(vs)	694(vs)	694(vs)
736(w)			734(m)	
	765(vs)			765(m)
		800(w)	797(m)	
	835(w)	833(w)	833(w)	
965(m)	966(w)	957(w)	958(w)	965(w)
975(m)	978(s)			
983(w)			982(w)	
	1006(m)			
	1026(w)	1026(w)	1026(w)	1024(w)
1037(w)	1039(w)			
1115(w)	1117(w)		1115(w)	

Table 35A-9-005. RbTiOPO₄. Raman modes [91Wat]. Roman numerals simply classify the frequency ranges. w: weak; m: medium; s: strong; v: very. ν : frequency [cm⁻¹] of Raman mode.

RTP	$A_1 x(zz)y$			$A_1 z(xx)y$			$A_1 x(yy)z$			$B_2 x(zy)z$			$B_1 x(zx)z$			$A_2 x(yx)z$		
	ν [cm ⁻¹]	HW	Amp	ν [cm ⁻¹]	HW	Amp.	ν [cm ⁻¹]	HW	Amp.	ν [cm ⁻¹]	HW	Amp.	ν [cm ⁻¹]	HW	Amp.	ν [cm ⁻¹]	HW	Amp.
I	51.0	1.1	vw				51.2	1.3	vvw	50.8	1.7	–	51.4	1.3	m	52.2	1.7	vs
				52.0	1.0	m												
	62.8	1.4	vvw	63.4	2.8	vw	56.8	2.9	vvw				56.2	1.7	ms			
	67.8	1.3	vvw	69.6	0.7	vw	63.0	1.3	w	65.6	3.1	vvw	63.0	0.5	w	61.0	1.8	m
	73.2	1.2	vvw	74.6	1.5	mw	69.8	0.9	mw				69.6	1.2	mw	66.6	0.8	m
				78.8	0.9	mw	74.4	2.0	vw				74.6	1.6	w			
	83.4	1.1	vw	84.2	1.3	s	78.4	0.9	w	77.8	1.0	mw	78.4	0.6	w	77.6	2.1	w
	98.4	0.8	vw	98.8	0.9	s	84.8	2.1	mw	86.0	2.3	vvw	86.0	1.3	ms	86.8	1.1	w
	106.8	0.8	mw	107.0	0.8	vs	100.6	1.0	vw				101.4	0.8	ms	107.0	0.9	vvs
							106.8	0.7	mw	104.8	1.9	ms						
II				121.0	1.2	w	111.8	2.1	w	112.4	2.9	m				120.6	1.3	ms
							128.2	1.8	w	120.4	1.2	m	128.8	1.4	vs			
	144.0	2.4	w	137.8	2.2	vvw				136.4	1.5	m				137.6	1.8	m
	161.4	1.6	mw	144.4	2.2	m	143.6	2.4	mw				143.4	2.3	w			
	170.8	2.7	vw	173.4	2.5	vw	161.6	1.7	s	164.2	1.9	vs	160.8	1.7	mw	163.6	2.3	s
										172.6	1.6	m	179.8	1.4	vs			
	198.4	3.5	vvw	198.8	2.1	vw							189.0	2.5	vs	192.8	2.4	ms
	206.2	3.0	w	205.4	2.8	mw	206.0	2.3	m	203.6	2.2	vvs						
	211.6	1.9	vs	213.2	1.8	s	213.0	2.2	vs	218.2	1.1	ms	213.4	2.1	ms	210.6	2.9	mw
										228.0	2.5	vs						
				238.0	2.1	w				235.8	2.2	mw				233.4	3.1	mw
				243.8	3.2	w	240.2	2.1	vw	243.6	4.0	w	241.0	3.1	m			

(continued)

Table 35A-9-005 (continued)

RTP	$A_1 x(zz)y$		$A_1 z(xx)y$		$A_1 x(yy)z$		$B_2 x(zy)z$		$B_1 x(zx)z$		$A_2 x(yx)z$	
	ν [cm ⁻¹]	HW Amp	ν [cm ⁻¹]	HW Amp.	ν [cm ⁻¹]	HW Amp.	ν [cm ⁻¹]	HW Amp.	ν [cm ⁻¹]	HW Amp.	ν [cm ⁻¹]	HW Amp.
III	263.4	3.4 mw	264.8	3.7 ms			265.0	3.1 vvs	256.6	2.5 s	259.6	3.2 ms
	270.8	2.8 vvs							263.6	3.1 mw	268.0	2.6 ms
	280.4	2.2 m	282.0	2.7 s	281.6	4.5 vs			276.0	3.8 vs		
	285.6	3.8 ms			289.2	3.7 ms	285.8	2.4 mw	281.4	2.3 ms		
	297.8	2.4 w	297.8	3.4 mw	298.0	1.1 w			285.6	4.0 vs	285.8	4.0 ms
IV	304.6	2.5 w	307.8	3.0 m			306.2	2.7 ms	298.2	1.9 m	298.0	2.6 s
					313.0	1.7 w	313.0	4.1 vs	304.0	3.6 m		
	322.8	6.1 vvw	320.6	2.1 vvw					313.8	3.9 m	311.8	3.4 m
					317.4	3.4 w	330.6	3.1 vvs	322.4	3.8 s		
			343.0	5.0 mw	331.0	3.6 vw			346.8	6.6 s	336.0	4.0 vvs
V	361.4	4.7 s	366.8	4.4 s	361.0	6.1 w	365.6	5.3 ms			348.2	2.6 vs
					369.0	3.8 vs	373.4	4.9 m				
	395.8	2.5 ms	395.4	2.3 s	394.4	2.1 s					392.0	3.2 mw
					397.6	3.7 mw			398.8	4.7 mw		
							407.6	2.0 m			408.8	2.3 w
VI	423.8	1.8 mw	421.8	2.1 vs			416.2	2.8 ms	415.2	1.7 vw		
									422.0	3.1 ms		
	464.8	6.0 –	477.4	3.6 ms	469.0	5.5 w	466.2	5.0 w	436.8	9.9 w		
			483.8	4.3 w	479.4	5.4 w	472.2	vw	468.0	5.6 w	477.0	7.9 w
					504.8	5.0 mw	488.4	4.2 vw				
			519.4	3.0 s					505.0	5.9 m	509.2	3.9 mw
	551.6	3.9 –	550.2	2.6 ms	550.0	2.7 mw						
			560.8	3.0 mw	558.6	2.3 –	559.0	3.3 m				
					564.8	2.0 w	567.4	2.0 w				
	575.8	1.8 –			574.2	2.0 vw			564.6	2.6 m		

(continued)

Table 35A-9-005 (continued)

RTP	$A_1 x(zz)y$		$A_1 z(xx)y$		$A_1 x(yy)z$		$B_2 x(zy)z$		$B_1 x(zx)z$		$A_2 x(yx)z$	
	ν [cm ⁻¹]	HW Amp	ν [cm ⁻¹]	HW Amp.	ν [cm ⁻¹]	HW Amp.	ν [cm ⁻¹]	HW Amp.	ν [cm ⁻¹]	HW Amp.	ν [cm ⁻¹]	HW Amp.
VIIa			588.2	3.1 vw								
			596.6	4.3 mw	595.2	5.1 w	595.0	4.4 vw	593.6	4.0 mw	594.2	2.8 vvw
	621.2	7.1 m	622.4	4.7 m	623.2	6.4 mw						
			629.4	7.1 mw			627.4	8.3 ms				
VIIb					638.4	6.9 m	632.8	5.2 ms	639.0	6.5 ms	631.4	6.7 –
											647.4	5.8 vw
	687.2	9.0 vs	693.4	7.7 vs			694.8	9.5 vvs			696.0	7.6 –
			749.2	7.1 vvs	723.4	8.8 vvs			720.2	9.0 m	723.8	8.8 vvw
VIII					792.6	8.7 w			793.2	9.1 vvs	796.0	9.2 s
					823.4	9.5 vw					816.8	6.1 ms
	833.4	6.9 –	834.0	5.3 mw	834.2	6.2 mw	833.2	6.4 w				
			958.6	3.9 w			956.6	4.2 vw			957.0	3.6 m
IX					964.6	5.4 m			969.4	3.1 s	968.0	4.2 ms
	966.0	4.6 vvw										
	983.0	3.3 vw	976.2	2.8 ms	981.4	2.9 vw	980.6	3.0 –	984.8	4.5 ms		
	990.4	2.7 –	986.4	6.3 m	989.8	2.5 –	995.8	3.0 vw			994.6	2.9 w
							1010.6	1.8 –				
			1017.6	2.3 w					1017.8	2.1 vw	1019.4	2.9 vvw
	1035.6	2.7 vw	1031.6	2.5 mw	1026.4	3.0 mw	1024.4	2.6 w	1026.4	3.2 mw		
					1079.0	3.2 w						
					1088.0	4.5 vw						
	1090.0	2.3 –	1101.6	1.6 –	1108.0	3.9 vw	1104.8	2.4 –	1087.4	5.1 w	1083.6	4.5 vvw
			1124.6	4.2 –			1113.0	3.8 vvw	1107.2	3.4 mw		
									1120.0	3.8 vvw		