

Table 33B-5-001. Rb_{1-x}(NH₄)_xH₂PO₄ (RADP, x = 0.50), Rb_{1-x}(ND₄)_xD₂PO₄ (DRADP, x = 0.50). Polar phonon parameters determined from far-infrared reflectivity [93Pet]. Parameter: *T*: ν : mode frequency [cm⁻¹], Γ : damping constant, $\Delta\kappa$: mode strength.

DRADP						RADP						Tentative
ν [cm ⁻¹]		Γ [cm ⁻¹]		$\Delta\kappa$		ν [cm ⁻¹]		Γ [cm ⁻¹]		$\Delta\kappa$		assignment ^{a)}
15 K	300 K	15 K	300 K	15 K	300 K	15 K	300 K	15 K	300 K	15 K	300 K	
B ₂ modes ($E \parallel c$)												
110	113	10	38	0.25	0.9							{ T(Rb-PO ₄) L(PO ₄)
184	202	15	71	0.35	1.2	157	127	35	60	1.3	1.0	
235	214	22	60	1.1	0.9	220	217	17	50	1.7	2.0	T(ND ₄ -PO ₄)
345	345	8	28	0.07	0.05	340	340	20	100	0.2	0.2	ν_2 (PO ₄)
485	481	24	60	0.23	0.25	470	470	150	250	0.4	0.8	ν_4 (PO ₄)
						75		180		2.8		Background
E modes ($E \perp c$)												
73	69	7	15	0.4	1.5	78	68	12	15	2.4	1.4	{ L(PO ₄) T(Rb-PO ₄)
105	105	40	80	0.65	1.3	120	–	40	–	1.6	0	
147	143	25	50	1.9	2.2	165	159	22	30	2.5	1.6	{ T(ND ₄ -PO ₄)
200	185	8	60	0.2	0.2	208	208	16	30	0.3	0.2	
230	218	33	90	1.1	1.9	238	238	14	80	0.5	0.7	
347	347	2	17	0.02	0.08	348	349	20	40	0.2	0.04	ν_2 (PO ₄)
390	392	22	45	0.4	0.38	397	405	21	140	0.2	1.2	ν_4 (PO ₄)
460	463	11	25	0.12	0.03	–	–	–	–	–	–	ν_2 (PO ₄)
518	520	25	30	0.25	0.25	540	544	16	25	0.1	0.2	ν_4 (PO ₄)
						165		300		15		Background

^{a)} L: libration; T: translation; ν_i : internal modes.

Table 33B-5-002. Rb_{1-x}(ND₄)_xD₂PO₄ (DRADP, x = 0.50). Frequencies [cm⁻¹] of observed Raman mode [95Yuz]. ^P: PO. ^N: ND₄. L: libration. *: main peaks for internal vibrations of PO₄. s: strong, w: weak, vw: very weak.

$Y(XX) Z = A_1 + B_1$		$Y(ZZ) X = A_1$		$Y(ZX) Z = E$		$Y(XY) Z = B_2$		Assignment
300 K	15 K	300 K	15 K	300 K	15 K	300 K	15 K	
80w		77vw		78	80	78vw		external translations
112w	114vw				108	112vw?	114?	
				124	132			L ^P
				166	174			
172	180				186	170	180	L ^N
	234	219	231	223	239		236	
	317		312					ν ₂ ^P
350*	349	352*	348	350	350	352	348	
380	383				382vw	382*	382	
	408				400		408	
450*	454				454	450*	454	ν ₄ ^P
				476*	468			
508	508	510	506		505	510	504	
					518			
540	542			530*	538	542	540	
	540		545vw		548		550	
700vw	700	700vw	706	706vw	718	700vw	702	γ(O–D)
	868		868		868		868	ν ₁ ^P
882s*	882s	882s*	882s	882w	882	882w	882	
					918			ν ₃ ^P
				932*	938			
968*		956	964					← δ(O–D)
990	982	988	981	978	978	980	980	
	1038					1050	1040	ν ₄ ^N
							1102	
1188	1104		1104	1090	1096		1102	ν ₂ ^N
	1186	1186	1186	1168	1186	1188w	1186	
						1120w	1228	
1360	1362				1366		1364	2γ(O–D)?
	1560							ν(O–D)
1760	1733			1760	1750	1760	1730	
	1838							
1990	1968			2000	1970	2005	1954	
2156	2166	2168	2168	2150	2150	2158	2162	ν ₂ ^N
2238	2238	2268	2238	2248	2240	2240	2238	
	2300		2310	2306	2318		2300	
2350	2350					2355	2352	ν ₃ ^N
		2390	2404	2416	2408			
2434	2448		2440		2448	2430	2448	

Table 33B-5-003. Rb_{1-x}(NH₄)_xH₂PO₄. Spin Hamiltonian parameters for AsO₄⁴⁻ [92Bab]. $T = \text{RT}$. \parallel and \perp : components are calculated using the field values for $\boldsymbol{H} \parallel \boldsymbol{c}$ and $\boldsymbol{H} \perp \boldsymbol{c}$.

x	A_{\parallel} [MHz]	A_{\perp} [MHz]	A_{iso} [MHz]	g_{\parallel}	g_{\perp}
1(ADP)	3281(2)	2946(2)	3057(2)	2.001(1)	2.001(1)
0.95	3276(2)	2945(2)	3055(2)	1.999(1)	2.001(1)
0.9	3275(2)	2941(2)	3053(2)	2.001(1)	2.002(1)
0.8	3272(2)	2939(2)	3050(2)	2.000(1)	2.001(1)
0.5	3262(2)	2934(2)	3043(2)	2.000(1)	2.002(1)
0 (RDP)	3231(2)	2922(2)	3025(2)	2.001(1)	2.003(1)