Table 40A-2-001. $RbHSO_4$. Structure of phase I [75Ash]. Fractional coordinates obtained by neutron diffraction and X-ray diffraction. $T = 23$ °C. See also Fig. 40A-2-001.

	Neutron diffraction	X-ray diffraction		Neutron diffraction	X-ray diffraction
Rb1 x	0.1231 (3)	0.1233 (2)	O14 x	0.1050 (6)	0.1031 (20)
y	0.1414 (12)	0.1405 (4)	y	0.4912 (17)	0.4893 (20)
z	0.4158 (3)	0.4160 (2)	z	0.1194 (7)	0.1185 (20)
Rb2 x	0.3748 (3)	0.3749 (2)	O21 x	0.4665 (4)	0.4662 (20)
y	0.7017 (12)	0.7018 (4)	y	0.6903 (15)	0.6914 (33)
z	0.3361 (3)	0.3360 (2)	z	0.0737 (4)	0.0709 (18)
S1 x	0.1257 (8)	0.1246 (5)	O22 x	0.4102 (5)	0.4064 (11)
y	0.2113 (27)	0.2171 (8)	y	0.9944 (17)	0.9963 (26)
z	0.1743 (8)	0.1741 (5)	z	0.1676 (5)	0.1652 (10)
S2 x	0.3728 (7)	0.3715 (5)	O23 x	0.2851 (4)	0.2848 (13)
y	0.7549 (29)	0.7614 (9)	y	0.8826 (16)	0.8838 (27)
z	0.0795 (7)	0.0787 (5)	z	−0.0166 (3)	−0.0171 (11)
O11 x	0.0322 (4)	0.0318 (10)	O24 x	0.3356 (4)	0.3392 (11)
y	0.1199 (17)	0.1096 (30)	y	0.5229 (16)	0.5205 (25)
z	0.1769 (4)	0.1790 (10)	z	0.1175 (4)	0.1167 (9)
O12 x	0.1410 (6)	0.1370 (10)	H1 x	0.1312 (9)	—
y	0.0164 (25)	0.0160 (30)	y	0.8081 (32)	—
z	0.0986 (6)	0.0955 (10)	z	0.1098 (8)	—
O13 x	0.2221 (4)	0.2223 (20)	H2 x	0.3778 (8)	—
y	0.2061 (21)	0.2032 (40)	y	0.1956 (25)	—
z	0.2735 (5)	0.2775 (20)	z	0.1388 (8)	—

Table 40A-2-002. $RbHSO_4$. Structure of phase I [75Ash]. Anisotropic temperature factors [$\cdot 10^4$ Å^2]. X-ray results are on the first line and neutron results on the second for each atom. U_{ij} is defined by Eq. (d) in Introduction.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Rb1	207(12)	243(9)	261(12)	6(7)	114(9)	–13(7)
	269(17)	375(30)	249(20)	–20(25)	122(15)	16(26)
Rb2	235(13)	297(8)	250(12)	9(8)	122(9)	11(8)
	306(19)	451(38)	291(21)	28(24)	180(15)	21(24)
S1	256(34)	143(17)	205(29)	–2(18)	134(25)	–20(17)
	309(43)	470(75)	285(49)	–66(60)	136(36)	13(62)
S2	178(31)	175(18)	202(28)	21(16)	88(24)	–5(16)
	244(35)	408(62)	282(48)	154(51)	128(34)	–26(56)
O11	228(92)	455(77)	335(97)	–65(69)	156(73)	–42(71)
	339(25)	494(41)	437(29)	–109(32)	211(22)	–66(35)
O12	488(109)	350(70)	239(83)	–166(67)	249(75)	–139(59)
	725(48)	605(72)	493(41)	–156(49)	457(35)	–155(47)
O13	404(141)	856(128)	409(134)	–117(96)	169(106)	–147(94)
	354(25)	983(71)	438(31)	–95(38)	138(22)	–98(42)
O14	1202(195)	129(62)	928(161)	47(83)	760(149)	217(78)
	1006(58)	254(40)	1101(64)	156(38)	721(48)	179(47)
O21	306(116)	530(91)	577(136)	153(75)	279(96)	52(83)
	313(24)	487(49)	405(28)	95(27)	199(22)	–6(31)
O22	391(98)	221(59)	195(73)	57(60)	85(67)	–11(54)
	433(29)	308(39)	297(29)	25(32)	118(23)	–78(33)
O23	236(91)	339(68)	108(70)	73(59)	–27(62)	26(54)
	340(23)	404(37)	269(22)	9(29)	117(18)	35(34)
O24	303(87)	222(57)	137(69)	–89(54)	74(62)	–36(48)
	420(28)	404(43)	365(28)	–62(31)	208(23)	37(35)
H1	–	–	–	–	–	–
	480(59)	532(91)	397(61)	19(65)	195(47)	–26(67)
H2	–	–	–	–	–	–
	491(52)	344(67)	390(58)	80(52)	220(46)	71(56)

Table 40A-2-003. $RbHSO_4$. Structure of phase I [75Ash]. Interatomic distances [Å] and angles [º] in sulfate ions. Translations are indicated in parantheses after the atom label.

Atom	Neutron	X-ray	Atom	Neutron	X-ray
S1–O11	1.43(1)	1.46(2)	O22–O23	2.43(1)	2.40(2)
–O12	1.54(2)	1.57(2)	–O24	2.37(1)	2.36(2)
–O13	1.41(1)	1.45(2)	O23–O24	2.40(1)	2.40(2)
–O14	1.48(2)	1.45(2)	O12–O14(*b*)	2.53(1)	2.54(2)
S2–O21	1.42(1)	1.46(3)	O22–O24(*b*)	2.62(1)	2.57(2)
–O22	1.58(1)	1.55(2)	O11–S1–O12	110(1)	107(1)
–O23	1.45(1)	1.44(2)	O11–S1–O13	114(1)	110(2)
–O24	1.44(2)	1.43(2)	O11–S1–O14	110(1)	113(2)
O11–O12	2.42(1)	2.43(3)	O12–S1–O13	109(1)	110(2)
–O13	2.37(1)	2.39(3)	O12–S1–O14	100(1)	100(1)
–O14	2.38(1)	2.42(3)	O13–S1–O14	114(1)	117(1)
O12–O13	2.39(1)	2.47(3)	O21–S2–O22	105(1)	108(1)
–O14	2.31(1)	2.30(2)	O21–S2–O23	113(1)	112(1)
O13–O14	2.41(1)	2.46(3)	O21–S2–O24	115(1)	111(1)
O21–O22	2.39(1)	2.43(3)	O22–S2–O23	106(1)	107(2)
–O23	2.40(1)	2.40(3)	O22–S2–O24	104(1)	105(1)
–O24	2.41(1)	2.38(2)	O23–S2–O24	112(1)	114(1)

Table 40A-2-004. $RbHSO_4$. Structure of phase I [75Ash]. Interatomic distances [Å] and angles [º] involving hydrogens obtained by neutron diffraction. T = 23 °C. Atoms are those in the same asymmetric unit unless otherwise indicated. A double prime denotes atoms obtained by a two fold operation, while a single prime denotes a glide operation. Translations are indicated in parentheses after the atom label.

O12–H1	0.99 (1)	O22–H2	1.04 (1)
O12–O14(*b*)	2.53 (1)	O22–O24(*b*)	2.62 (1)
H1···O14(*b*)	1.54 (2)	H2···O24(*b*)	1.59 (1)
∠ O12–H1···O14(*b*)	174 (1)	∠ O22–H2···O24(*b*)	169 (1)
∠ S1–O12–H1	111 (1)	∠ S2–O22–H2	114 (1)
H1–Rb1′(–*a*)	3.50 (1)	H2–Rb1″(–*c*)	3.52 (1)
–Rb1″(–*c*)	3.56 (1)	–Rb2(–*a*)	3.73 (1)
–Rb1″(*b*–*c*)	3.80 (1)	–Rb2	3.76 (1)
–Rb2	3.41 (1)	–Rb2′	3.38 (1)

Table 40A-2-005. $RbHSO_4$. Structure of phase I [75Ash]. Distances [Å] between rubidium and oxygen at 23 °C. Atoms are those in the same asymmetric zone unless otherwise indicated. A double prime denotes atoms obtained by a twofold screw operation, while a single prime denotes a glide operation. Translations are indicated in parentheses after the atom label.

Atoms	Neutron	X-ray	Atoms	Neutron	X-ray
Rb1–O11	3.07(1)	3.05(2)	Rb2–O21′(*a*)	2.99(1)	3.00(2)
–O11′	2.93(1)	2.90(2)	–O21′(*a*–*b*)	3.07(1)	3.07(2)
–O11′(–*b*)	3.09(1)	3.12(2)	–O21″(*b*)	3.10(1)	3.06(3)
–O12″	3.03(1)	3.02(2)	–O22	3.10(1)	3.10(2)
–O13	3.10(1)	3.05(3)	–O22′(*a*–*b*)	3.26(1)	3.30(2)
–O14′(–*b*)	3.12(1)	3.10(3)	–O23″(*b*)	3.08(1)	3.07(2)
–O14″	3.22(1)	3.22(2)	–O24	3.10(1)	3.13(2)
–O23″	3.14(1)	3.14(1)	–O13	3.00(1)	2.98(2)
–O23″(*b*)	2.98(1)	2.97(2)	–O13(*b*)	2.97(1)	2.99(2)
–O24	3.07(1)	3.08(2)			

Table 40A-2-006. $RbDSO_4$. $|eQ\phi_{ii}/h|$ of ^{87}Rb [74Kas]. Principal values of the nuclear quadrupole coupling tensor and their direction cosines with respect to the crystallographic axes a', b', c'^*. c'^* is perpendicular to the $a'b'$-plane. A, B and A_1, A_2, B_1, B_2 correspond to different ^{87}Rb sites above and below Θ_t, respectively.

T °C	$\lvert eQ\phi_{ii}/h\rvert$ kHz		Direction cosine			$\lvert eQ\phi_{ii}/h\rvert$ kHz		Direction cosine		
			a'	b'	c'^*			a'	b'	c'^*
18	A	4006	0.890	0.492	0.154	B	3652	0.913	0.216	0.354
		3038	0.453	−0.795	−0.404		3272	0.005	−0.854	0.521
		968	0.051	−0.429	0.902		380	−0.407	0.474	0.781
−50	A_1	6323	0.879	0.473	0.054	B_1	4118	0.995	−0.031	0.093
		4687	0.458	−0.807	−0.372		4472	−0.073	−0.866	0.494
		1636	0.132	−0.352	0.927		354	−0.065	0.499	0.864
	A_2	2676	0.859	0.384	0.344	B_2	3795	0.836	0.374	0.401
		2583	0.485	−0.826	−0.285		2037	0.432	−0.900	0.061
		93	−0.174	−0.412	0.895		1758	−0.338	0.224	0.914

Table 40A-2-007. $RbDSO_4$. $eQ\phi_{ii}/h$ of ^2D [74Kas]. Principal values of the nuclear quadrupole coupling tensor and their direction cosines with respect to the crystallographic axes a', b', c'^*. c'^* is perpendicular to the $a'b'$-plane. T = 20 °C. See also caption of Table 40A-2-008.

	$eQ\phi_{ii}/h$ kHz	Direction cosine				$eQ\phi_{ii}/h$ kHz	Direction cosine		
		a'	b'	c'^*			a'	b'	c'^*
D_1	−171.5	−0.106	±0.970	0.218	D_2	−167.6	0.395	±0.908	0.143
	96.3	±0.989	0.081	±0.120		92.3	±0.802	−0.264	∓0.535
	75.2	−0.099	∓0.228	0.968		75.3	0.448	∓0.326	0.832

Table 40A-2-008. $RbDSO_4$. $eQ\phi_{ii}/h$ of ^2D [75Kas]. Principal values of the nuclear quadrupole coupling tensor and their direction cosines with respect to the crystallographic axes a', b', c'^*. c'^* is perpendicular to the $a'b'$-plane. T = –120 °C. Two crystallographically inequivalent sites in the paraelectric (P) phase result in four sites in the ferroelectric phase. D_1 in the P-phase splits into D_1 and D_1', D_2 into D_2 and D_2'.

	$eQ\phi_{ii}/h$ kHz	Direction cosine				$eQ\phi_{ii}/h$ kHz	Direction cosine		
		a'	b'	c'^*			a'	b'	c'^*
D_1	−192.1	−0.002	±0.982	0.177	D_2	−166.4	0.382	±0.911	0.157
	110.5	±0.999	−0.001	±0.015		92.8	±0.789	−0.233	∓0.568
	81.6	−0.015	∓0.177	0.984		73.6	0.481	∓0.341	0.808
D_1'	−165.2	−0.307	±0.933	0.190	D_2'	−168.2	0.456	±0.882	0.119
	92.3	±0.886	0.207	±0.416		94.3	±0.703	−0.275	∓0.656
	72.9	−0.348	∓0.296	0.889		73.9	0.545	∓0.383	0.745

Table 40A-2-009. $RbHSO_4$. ^{85}Rb nuclear quadrupole frequencies, coupling constants and asymmetry parameters at 150 K [93Abr].

$\nu_{1/2-3/2}$ [kHz]	$\nu_{3/2-5/2}$ [kHz]	eQV_{ZZ}/h [kHz]	η
1155	1530	5480	0.67
1320	2270	7750	0.37
2310	2740	10020	0.80
2840	4245	14870	0.53