Table 40A-7-001. $RbHSeO_4$. Structure of phase II [78Was]. Fractional coordinates of atoms in the unit cell.

	x	*y*	*z*
Rb (1)	0.0840 (2)	0.7207 (8)	0.1585 (5)
Rb (2)	0.2495 (2)	0.3045 (10)	0.7583 (5)
Rb (3)	0.4151 (2)	0.8914 (8)	0.1601 (5)
Se (1)	0.0830*)	0.8400*)	0.6700*)
Se (2)	0.2512 (2)	0.2992 (9)	0.2469 (4)
Se (3)	0.4175 (2)	0.7744 (6)	0.6701 (4)
O (1)	0.1476 (15)	0.7367 (57)	0.7924 (30)
O (2)	0.0213 (12)	0.9862 (54)	0.7806 (35)
O (3)	0.1218 (11)	0.1006 (47)	0.5328 (31)
O (4)	0.0589 (13)	0.5838 (43)	0.5347 (30)
O (5)	0.3171 (11)	0.4325 (47)	0.1262 (27)
O (6)	0.1895 (11)	0.1906 (47)	0.1325 (28)
O (7)	0.2818 (11)	0.0391 (42)	0.3773 (27)
O (8)	0.2217 (10)	0.5622 (45)	0.3857 (26)
O (9)	0.3842 (13)	0.5224 (46)	0.5326 (31)
O (10)	0.3555 (11)	0.8768 (50)	0.7942 (28)
O (11)	0.4482 (13)	0.0300 (47)	0.5388 (30)
O (12)	0.4848 (14)	0.6406 (60)	0.7734 (39)

*) Fixed parameters.

Table 40A-7-002. $RbHSeO_4$. Structure of phase II [80Was]. T = 387 K. Fractional coordinates and anisotropic temperature parameters [$\cdot 10^{-2}$ Å]. U_{ij} is defined by Eq. (d) in Introduction.

Atom	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Rb2	0.0	0.0	0.5132(2)	1.94	2.62	2.32	0.63	0.0	0.0
Rb3	0.1651(1)	0.5825(3)	0.9142(3)	1.86	2.48	2.57	0.18	–0.02	–0.01
Se2	0.0	0.0	0.0*	1.26	1.46	1.65	–0.31	0.0	0.0
Se3	0.1675(1)	0.4691(2)	0.4234(2)	1.41	1.37	1.96	0.37	–0.39	–0.32
O5	0.0611(4)	0.1094(22)	–0.1159(10)	2.32	2.61	2.73	–0.97	0.83	–0.53
O7	0.0256(6)	–0.2688(23)	0.1372(9)	2.44	2.75	2.06	1.17	0.78	–0.07
O9	0.1330(5)	0.2101(21)	0.2868(11)	2.28	2.47	3.25	0.41	–0.96	0.22
O10	0.1072(5)	0.5770(22)	0.5519(12)	3.61	3.07	3.16	1.14	–0.82	0.77
O11	0.1939(6)	0.7223(20)	0.2877(11)	1.92	1.18	2.66	–0.99	0.93	0.04
O12	0.2283(42)	0.3152(25)	0.5379(13)	4.51	4.78	4.36	2.31	–0.91	0.46

* Fixed to define the origin on the *c* axis.

Table 40A-7-003. $RbHSeO_4$. Structure of phase II [80Was]. T = 387 K. Interatomic distances [Å] and bond angles [°]. Prime denotes atoms in the position $-x, -y, z$.

Se2–O7	1.71(2) Å	O7–Se2 –O5	110.9(3)°
–O5	1.56(1)	O7– –O7′	104.2(4)
		O5– –O7′	109.9(3)
		O5– –O5′	110.8(3)
Se3–O9	1.72(2)	O9–Se3–O10	107.9(3)
–O10	1.61(1)	O9– –O11	103.3(4)
–O11	1.64(2)	O9– –O12	107.3(4)
–O12	1.64(1)	O10– –O11	112.6(3)
		O10– –O12	110.0(4)
		O11 –O12	115.2(3)

Table 40A-7-004. $RbHSeO_4$. Structure of phase III [89Mak]. T = 293 K. Fractional coordinates and thermal motion parameters.

Atom	x	y	z	B_{eff} [Å^2]
Rb(1)	–0.0002(1)	0.0027(5)	0.4881(3)	2.33(2)
Rb(2)	0.16535(9)	0.5788(5)	0.0852(3)	2.32(3)
Rb(22)	0.83461(9)	0.4195(5)	0.0879(3)	2.33(2)
Se(1)	0.00129(7)	0.0101(3)	0.0000(2)	1.53(2)
Se(2)*	0.16745	0.6983	0.5768	1.70(2)
Se(22)	0.83259(7)	0.2995(3)	0.5776(2)	1.73(2)
O(1)	0.0302(1)	0.2884(5)	0.8695(3)	2.22(3)
O(11)	0.9703(1)	0.7163(5)	0.8603(3)	2.25(3)
O(2)	0.0628(1)	0.9378(7)	0.1190(3)	2.58(4)
O(22)	0.9359(1)	0.0499(7)	0.1160(3)	2.68(4)
O(3)	0.1942(1)	0.4711(5)	0.7096(4)	2.50(3)
O(33)	0.8055(1)	0.5281(5)	0.7113(4)	2.52(3)
O(4)	0.2303(2)	0.9011(7)	0.4704(4)	3.26(5)
O(44)	0.7700(1)	0.0946(7)	0.4690(4)	3.27(5)
O(5)	0.1318(1)	0.9202(5)	0.7149(4)	2.64(4)
O(55)	0.8680(1)	0.0797(5)	0.7146(4)	2.64(4)
O(6)	0.1045(1)	0.5314(7)	0.4522(4)	3.00(4)
O(66)	0.8960(1)	0.4621(7)	0.4560(4)	2.91(4)
H(1)	0.9964(2)	0.5482(9)	0.8718(6)	2.73(6)
H(2)	0.1577(2)	0.1364(10)	0.7083(7)	3.23(7)
H(22)	0.8417(3)	0.8637(10)	0.7083(7)	2.27(7)

* Position of Se(2) atom fixed during refinement.

Table 40A-7-005. $RbDSeO_4$ (92 % deuterated). Structure at RT [82Was]. Fractional coordinates and mean square displacements [$\cdot 10^{-2}$ Å^2].

Atom	*x*	*y*	*z*	$\overline{u^2}$
Se	0.12637(3)	0.23157(8)	0.54024(5)	1.28(1)
Rb	0.12224(3)	0.31597(9)	0.05116(5)	2.32(1)
O(1)	0.2173(3)	0.0806(9)	0.4309(5)	3.62(1)
O(2)	0.0313(3)	0.3417(9)	0.4202(4)	2.67(1)
O(3)	0.1696(3)	0.4823(8)	0.6730(5)	2.51(1)
O(4)	0.0745(3)	–0.0236(8)	0.6806(3)	2.04(1)
D	0.109(6)	–0.225(9)	0.678(6)	6.8(19)

Table 40A-7-006. $RbDSeO_4$ (92 % deuterated). Structure at RT [82Was]. Interatomic distances [Å] and bond angles [°] of SeO_4 tetrahedra.

Se–O(1)	1.592(4)
–O(2)	1.603(3)
–O(3)	1.623(4)
–O(4)	1.714(3)
mean	1.633(7)
O(1)–Se–O(2)	114.1(2)
O(1)– –O(3)	112.1(2)
O(1)– –O(4)	107.8(2)
O(2)– –O(3)	112.6(2)
O(2)– –O(4)	105.3(1)
O(3)– –O(4)	104.0(2)

Table 40A-7-007. $RbHSeO_4$. Unit cell parameters at several temperatures [79Pie].

T	*a*	*b*	*c*	α	*β*	*γ*
K	Å			deg		
298.78	19.35927	4.61883	7.57104	90.648	89.792	90.720
358.48	19.42285	4.62636	7.59484	90.563	89.820	90.699
370.61	19.43649	4.62783	7,59866	89.927	89.955	90.689
381.88	19.44872	4.62932	7.60458	89.995	89.989	90.695
395.64	19.46457	4.63110	7.61094	89.988	89.998	90.693

Table 40A-7-008. $RbHSeO_4$. Raman frequency shifts ($\Delta\nu/c$) [cm^{-1}] at 20 K and 300 K [82Car]. vw: very weak, sh: shoulder.

20 K	300 K	Assignment
2620	2650	ν(OH)A
2250	2300	ν(OH)B
2200		
1695	1620	ν(OH)C
1667		$2\nu_1$ (?)
1604		
1570		$\nu_1 + \nu_3$
1256	1230	δ(OH)
1233		
959 (sh)		ν_3 (E in C_{3v}) and γ(OH) (?)
955	954	
920 (sh)		
913	916	
904 (sh)	908 (sh)	
844 (vw)		$2\nu_4$
821	829	ν_1
802	816 (sh)	
750 (sh)	745 (sh)	ν_3 (A_1 in C_{3v})
739	733	
430	420	ν_4
420		
405	405	
397	397	
394		
391		
373	375	
357	353	ν_2
331	334	
326		
317	320	
305	308	
175 (sh)		$HSeO_4^-$ libration
163		
158	160	
140		
136		
111		translation or libration
100	98	
89		
76	77	translation
	74	
67		
64	62	
54	55	
49	49	
46		
36	35	

Table 40A-7-009. $RbHSeO_4$, NH_4HSeO_4. Chemical shift parameter of ^{77}Se [83Roz]. $\Delta\sigma = \sigma_{zz} - (\sigma_{xx} + \sigma_{yy})/2$. $\eta = (\sigma_{yy} - \sigma_{xx})/(\sigma_{zz} - \bar{\sigma})$. σ_{ii}: principal values of chemical shift tensor. $\bar{\sigma}$: average of the three principal values.

	T [K]	Nuclei	Anisotropy $\Delta\sigma$	Asymmetry parameter η
NH_4HSeO_4	293	Se(1)	206(4)	0.98(1)
		Se(2)	−326(4)	0.44(1)
		Se(1)	−286(4)	0.43(1)
	202	Se(2)	−326(4)	0.51(1)
		Se(3)	−326(4)	0.50(1)
$RbHSeO_4$	388	Se(1)	229(6)	0.94(1)
		Se(2)	−329(6)	0.45(1)
		Se(1)	−322(6)	0.49(1)
	293	Se(2)	−322(6)	0.48(1)
		Se(3)	−323(6)	0.50(1)