Table 31A-4-001. $RbH_3(SeO_3)_2$. Crystal structure of phase I [77Tel]. Fractional coordinates [$\cdot 10^{-5}$] at 25 °C.

Atom	x	y	z
Se (1)	21603 (16)	39522 (5)	29592 (16)
Se (2)	73074 (17)	24230 (5)	16852 (15)
O (1)	19248 (30)	42042 (9)	02792 (26)
O (2)	50871 (27)	22527 (10)	32176 (38)
O (3)	49199 (22)	42598 (8)	33834 (29)
O (4)	77270 (27)	33469 (8)	18980 (28)
O (5)	07888 (26)	46154 (8)	42234 (31)
O (6)	95431 (29)	20776 (10)	31866 (40)
Rb	26060 (20)	08290 (6)	23376 (21)
H (1)	27392 (52)	46900 (16)	−00433 (50)
H (2)	97911 (55)	23704 (18)	45659 (73)
H (3)	60320 (52)	38474 (18)	28169 (51)

Table 31A-4-002. $RbH_3(SeO_3)_2$. Crystal structure of phase I [77Tel]. Anisotropic temperature parameters and the root-mean-square components R_i [$\cdot 10^{-3}$ Å] of thermal displacement along the ellipsoids axes. $T = 25$ °C. b_{ij} is defined by Eq. (b) in Introduction.

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}	R_1	R_2	R_3
Se (1)	1311 (24)	0091 (2)	1059 (22)	−0014 (5)	−0027 (17)	−0017 (5)	121 (2)	145 (2)	153 (1)
Se (2)	1443 (24)	0130 (3)	0947 (21)	−0015 (6)	0096 (19)	−0037 (5)	132 (2)	148 (1)	163 (1)
O (1)	2447 (45)	0192 (4)	1169 (35)	−0259 (12)	−0399 (33)	0076 (9)	144 (2)	149 (2)	234 (2)
O (2)	1605 (39)	0228 (5)	2448 (53)	−0209 (11)	0703 (40)	−0163 (13)	139 (2)	181 (2)	250 (2)
O (3)	1314 (34)	0148 (4)	1891 (42)	−0004 (10)	−0275 (30)	−0066 (10)	145 (2)	155 (2)	200 (2)
O (4)	1701 (38)	0129 (3)	1965 (41)	0018 (9)	0462 (35)	0025 (9)	145 (2)	158 (2)	211 (2)
O (5)	1427 (34)	0163 (4)	2208 (45)	−0019 (9)	0351 (34)	−0238 (11)	135 (2)	157 (2)	229 (2)
O (6)	1778 (41)	0180 (4)	3036 (62)	0219 (11)	−0772 (45)	−0134 (15)	135 (2)	183 (3)	264 (3)
Rb	1535 (29)	0165 (3)	1522 (30)	0028 (8)	0071 (25)	0043 (6)	159 (2)	164 (2)	179 (2)
H (1)	2281 (73)	0227 (7)	2010 (68)	−0059 (21)	−0115 (62)	0081 (18)	183 (3)	196 (4)	214 (4)
H (2)	2295 (78)	0251 (9)	3559 (130)	0062 (23)	−0675 (88)	0121 (30)	180 (4)	210 (4)	276 (5)
H (3)	2227 (72)	0272 (9)	1941 (74)	−0135 (22)	−0360 (62)	0113 (22)	179 (4)	188 (4)	234 (4)

Table 31A-4-003. $RbH_3(SeO_3)_2$. Crystal structure of phase I [77Tel]. Interatomic distances [Å] and angles [°]. T = 25 °C. Atoms outside the asymmetric unit carry a subscript which indicates how the atomic parameters can be derived from those of the asymmetric unit. The first three digits code the lattice translation (the asymmetric unit is in cell 555), and the fourth digit specifies the symmetry operation: 1: x, y, z; 2: $1/2 - x, -y, 1/2 + z$; 3: $1/2 + x, 1/2 - y, -z$; 4: $x, 1/2 + y, 1/2 - z$.

Covalent bonds			
O–Se–O	O–Se	Se–O	∢O–Se–O
O (1)–Se (1)–O (3)	1.741 (2)	1.745 (2)	98.0 (1)
O (1)–Se (1)–O (5)	1.741 (2)	1.644 (2)	103.6 (1)
O (3)–Se (1)–O (5)	1.745 (2)	1.644 (2)	99.2 (1)
O (2)–Se (2)–O (4)	1.655 (2)	1.682 (2)	104.7 (1)
O (2)–Se (2)–O (6)	1.655 (2)	1.737 (2)	103.1 (1)
O (4)–Se (2)–O (6)	1.682 (2)	1.737 (2)	101.3 (1)

Ionic bonds	
Rb–O $(1)_{5553}$	3.036 (2)
–O (2)	2.998 (2)
–O $(3)_{4563}$	3.116 (2)
–O $(3)_{6454}$	3.207 (2)
–O $(4)_{4553}$	3.034 (2)
–O $(5)_{5563}$	2.968 (2)
–O $(5)_{5454}$	3.120 (2)
–O $(6)_{4551}$	2.931 (2)

Hydrogen bonds			
O–H···O	O–H	H···O	O···O
O (1)–H (1)···O $(5)_{5642}$	1.017 (3)	1.589 (3)	2.599 (2)
O (6)–H (2)···O $(2)_{5563}$	1.020 (5)	1.552 (5)	2.570 (3)
O (3)–H (3)···O (4)	1.052 (3)	1.464 (3)	2.512 (2)
Z–O–H···O–W	∢Z–O–H	∢O–H···O	∢H···O–W
Se (1)–O (1)–H (1)···O (5)–Se (1)	112.1 (2)	172.1 (3)	115.9 (2)
Se (2)–O (6)–H (2)···O (2)–Se (2)	112.5 (2)	174.4 (4)	121.7 (2)
Se (1)–O (3)–H (3)···O (4)–Se (2)	108.9 (2)	173.0 (3)	122.3 (2)

Table 31A-4-004. $RbH_3(SeO_3)_2$. Direction cosines and the principal values of the EFG tensor of ^{87}Rb at 13 °C and –155.5 °C [79Tak]. See also Fig. 31A-4-020, Fig. 31A-4-021. Four inequivalent Rb sites A_1, A_2, B_1, B_2 were observed in the ferroelectric phase.

T °C		$\lvert eQ\phi_{ii}/h\rvert$	Direction cosine with respect to		
		kHz	*a*	*b*	*c*
13.0		5130	±0.299	±0.359	0.884
		3832	±0.789	0.615	∓0.017
		1298	0.538	0.702	∓0.467
−155.5	A_1	6129	−0.349	−0.455	0.819
		5566	−0.775	0.631	0.020
		563	0.526	0.628	0.573
	A_2	5151	−0.275	−0.379	0.884
		2968	0.119	0.898	0.423
		2183	0.954	−0.221	0.202
	B_1	5404	0.239	0.417	0.877
		4412	−0.811	0.583	−0.056
		992	0.535	0.697	−0.048
	B_2	5975	0.393	0.410	0.823
		3605	−0.589	0.800	−0.118
		2370	0.707	0.438	−0.555

Table 31A-4-005. $RbD_3(SeO_3)_2$. Principal values and the direction cosines of EFG tensor of deuterons at 14 °C [79Shi]. See also Fig. 31A-4-023, Fig. 31A-4-024.

	$eQ\phi_{ii}/h$	Direction cosine with respect to		
	kHz	*a*	*b*	*c*
D (1)	− 72.25	0.3106	0.0220	0.9503
	− 88.83	0.8194	−0.5129	−0.2560
	161.08	0.4817	0.8582	−0.1773
D (2)	− 65.02	0.7649	0.5992	−0.2364
	− 84.58	−0.6299	0.6192	−0.4689
	149.60	−0.1346	0.5076	0.8510
D (3)	− 48.46	0.7553	−0.6066	−0.2481
	− 71.19	−0.0302	−0.4105	0.9114
	119.65	0.6547	0.6809	0.3284

Table 31A-4-006. $RbH_3(SeO_3)_2$. Principal values and their direction cosines of **D** tensor of Cr^{3+} [82Tak].

Principal values [$\cdot 10^2$ Am^{-1}]		Direction cosines		
		l	*m*	*n*
D_x	80(16)	0.515	−0.071	0.855
D_y	1400(16)	−0.107	0.983	0.146
D_z	−1480(16)	0.851	0.167	−0.499