Table 31A-2-001. $NaH_3(SeO_3)_2$. Unit cell parameters of phases I and II [73Mik].

	Phase I (at 298 K)	Phase II (at 183 K)
a'	10.33_8 Å	20.32_0 Å
b'	4.84_0 Å	9.59_2 Å
c'	5.77_5 Å	5.75_9 Å
α'	90°00′	89°53′
β'	91°10′	91°07′
γ'	90°00′	90°20′

Table 31A-2-002. $NaH_3(SeO_3)_2$. Crystal structure of phase I [70Kap]. Fractional coordinates at RT. Parameters listed for $H_d(1)$ are obtained on the assumption that the H(1) atom is disordered. The coordinates refer to the a', b', c' axial system.

	x	y	z
Na	0	0	0
Se	0.1691 (2)	0.3861 (6)	0.5060 (4)
	0.1691	0.3850	0.5068
O (1)	0.4473 (4)	0.6904 (10)	0.1257 (6)
	0.4487	0.6948	0.1264
O (2)	0.6443 (3)	0.2072 (9)	0.2877 (6)
	0.6410	0.2015	0.2975
O (3)	0.3071 (3)	0.2067 (9)	0.4509 (6)
	0.3111	0.1980	0.4365
H (1)	0	0	1/2
$H_d(1)$	0.0180 (33)	0.0205 (199)	0.4851 (92)
H (2)	0.1721 (7)	0.4919 (21)	0.9152 (15)

Table 31A-2-003. $NaH_3(SeO_3)_2$. Crystal structure of phase I [70Kap]. Anisotropic temperature parameters. B_{ij} is defined by Eq. (a) in Introduction, referring to the a', b', c' axial system. For explanation of $H_d(1)$, see caption of Table 31A-2-002.

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
	10^{-4}					
Na	16 (7)	137 (4)	69 (2)	− 20 (16)	0 (11)	18 (31)
Se	38 (2)	147 (12)	93 (6)	− 7 (5)	− 2 (3)	7 (10)
O (1)	44 (3)	220 (22)	49 (9)	56 (8)	−18 (5)	− 13 (16)
O (2)	40 (3)	129 (19)	45 (8)	28 (8)	10 (5)	13 (14)
O (3)	30 (3)	149 (18)	70 (10)	17 (7)	12 (5)	38 (15)
H (1)	90 (12)	497 (77)	189 (31)	116 (31)	−45 (20)	− 47 (54)
H_d (1)	9 (33)	425 (272)	149 (103)	25 (100)	24 (46)	9 (152)
H (2)	66 (7)	634 (65)	206 (23)	90 (20)	15 (12)	144 (42)

Table 31A-2-004. $NaH_3(SeO_3)_2$. Crystal structure of phase I [70Kap]. Interatomic distances and angles. For explanation of $H_d(1)$, see caption of Table 31A-2-002. Atom with primed number is related to basis atom by an inversion center.

(a) involving oxygen atoms about the sodium ion			
Distances	[Å]	Angles	[deg]
Na–O (1)	2.407 (4)	O (1)–Na–O (2)	84.2 and 95.8 (2)
Na–O (2)	2.413 (4)	O (1)–Na–O (3)	87.0 and 93.0 (2)
Na–O (3)	2.462 (4)	O (2)–Na–O (3)	83.7 and 96.3 (2)
(b) involving selenite group			
Distances	[Å]	Angles	[deg]
Se–O (1)	1.700 (5)	O (1)–Se–O (2)	99.3 (3)
Se–O (2)	1.716 (5)	O (1)–Se–O (3)	102.7 (3)
Se–O (3)	1.707 (5)	O (2)–Se–O (3)	100.6 (3)
(c) involving hydrogen bonds			
Distances	[Å]	Angles	[deg]
O (1)–H (1)	1.301 (5)	O (1)–H (1)–O (1)	180
O (1)–O (1′)	2.602 (9)	O (2)–H (2)–O (3)	176.1 (9)
O (2)–H (2)	1.24 (1)		
O (3)–H (2)	1.31 (2)		
O (2)–O (3)	2.556 (6)		
O (1)–H_d(1)	1.11 (8)		
O (1′)–H_d(1)	1.50 (8)	O (1)–H_d(1)–O (1′)	170 (4)

Table 31A-2-005. $NaHD_2(SeO_3)_2$ and $NaH_2D(SeO_3)_2$. Crystal structures of phase I. Fractional coordinates and temperature parameters. The temperature parameters are defined by Eq. (e) in Introduction. Compound I: $NaHD_2(SeO_3)_2$ [74Noz], II: $NaH_2D(SeO_3)_2$ [75Noz]. The coordinates refer to the a', b', c' axial system [59Pep1].

Atom	Compound	x	y	z	B, Å^2	Multiplicity of the position
Na	I	0	0	0	1.04	2
	II	0	0	0	1.16	2
Se	I	0.1692	0.3841	0.5056	1.45	4
	II	0.1690	0.3850	0.5061	1.38	4
O 1	I	0.4466	0.6902	0.1253	1.54	4
	II	0.4471	0.6910	0.1256	1.63	4
O 2	I	0.6440	0.2078	0.2876	1.16	4
	II	0.6443	0.2075	0.2876	1.29	4
O 3	I	0.3077	0.2098	0.4509	1.25	4
	II	0.3071	0.2063	0.4510	1.18	4
H 1 [a])	I	0	0	$^1/_2$	2.65	1.65
	II	0	0	$^1/_2$	2.74	1.76
H 2 [a])	I	0.1734	0.4995	0.9144	2.96	4.36
	II	0.1751	0.5000	0.9122	2.69	4.26

[a]) The rate of substitution of H for D at site I is different from the rate at site II.

Table 31A-2-006. $XH_3(SeO_3)_2$, $XD_3(SeO_3)_2$, X = Na, K, Rb, Cs. Θ, $d\Theta/dp$ [71Shi].

Material	$NaH_3(SeO_3)_2$	$NaD_3(SeO_3)_2$	$KH_3(SeO_3)_2$	$KD_3(SeO_3)_2$	$RbH_3(SeO_3)_2$	$CsH_3(SeO_3)_2$
$\frac{d\Theta}{dp}$ [deg Pa^{-1}]	−1.1 (2)	−1.7 (1)	− 5.3 (4)	− 5.4 (2)	7.1 (6)	0.7 (1)
Θ [°C]	−78.8	−5.6	−58.8	−19.2	−113	−124

Table 31A-2-007. $NaH_3(SeO_3)_2$. Piezoelectric constants [$\cdot 10^{-11}$ C N^{-1}] at –80 °C [75Sch]. Primed quantities are coefficients in the coordinate system rotated by 45° around the $y\,(d'_{23})$ and $x\,(d'_{12})$ axis. x: direction perpendicular to c' and b' axes; $y = b'$ axis.

$d_{11} = 1.6$	$d_{21} = -0.3$
$d_{12} = 3.4$	$d_{22} = 5.5$
$d_{13} = -0.6$	$d_{23} = 0.9$
$d'_{12} = -0.6$	$d'_{23} = 1.0$
$d_{14} = -4.0$	$d_{25} = 1.7$

Table 31A-2-008. $NaH_3(SeO_3)_2$. Frequencies and assignments of vibrational modes at –196 °C [65Kha]. $10^2\ m^{-1}$ is equal to $3 \cdot 10^{10}$ Hz.

Frequency of absorption maxima [$10^2\ m^{-1}$]	Assignment	Frequency of absorption maxima [$10^2\ m^{-1}$]	Assignment
2800 v.b.	O–H···O (st.)	770, 755, 730	$\nu_3''HSeO_3^-$
2500, 2460, 2400, 2300	v.b. O–H···O (st.)	705, 694, 690	$\nu_3'H_2SeO_3$
1302, 1290, 1270	O–H···O in-plane bend	647, 633, 622	$\nu_3''H_2SeO_3$ and $\nu_1HSeO_3^-$
1245, 1235, 1225	O–H···O in-plane bend	478, 464, 438	$\nu_2HSeO_3^-$
1005, 990, 975	O–H···O out-of-plane bend	430, 407	$\nu_2H_2SeO_3$
		382	$\nu_4'H_2SeO_3$
950, 917, 907	O–H···O out-of-plane bend	375, 358	$\nu_4''H_2SeO_3$
		350, 348	$\nu_4'HSeO_3^-$
867, 857, 848	$\nu_3'HSeO_3^-$	334, 320, 317	$\nu_4''HSeO_3^-$
827, 812, 804	$\nu_1H_2SeO_3$		

v.b. = very broad; st. = stretching.

Table 31A-2-009. $Na(D_xH_{1-x})_3(SeO_3)_2$. $\Delta\nu$ vs. x [77Fed]. Frequencies of lattice modes below 300 cm^{-1} at RT obtained from Raman scattering spectra. Parameter x: concentration of deuterium. 1 cm^{-1} is equal to $3 \cdot 10^{10}$ Hz.

Symmetry type	Deuterium concentration in crystal, x				
	0	0.18	0.22	0.62	0.96
	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}
B_g	57	57	57	56	57
A_g	70	70	69	69	70
B_g	92	92	91	91	92
B_g	112	112	111	111	112
A_g	113	113	112	112	112
A_g	125	125	125	124	123
A_g	133	132	131	132	133
B_g	156	149	147	145	143
B_g	159	158	155	154	154
A_g	206	—	—	—	212
B_g	252	≈250	≈250	≈250	250
A_g	278	—	—	—	264

Table 31A-2-010. $NaD_3(SeO_3)_2$. Deuteron e^2qQ/h, η and relative intensity [69Sod]. In phase I two pairs of DMR lines, D_a and D_b were observed. Below Θ_t, D_a splits into 2 lines, D_b into 4 lines.

	e^2Qq/h [kHz]	η	Relative intensity
298 K			
D_a	145.5 (4)	0.156 (4)	1
D_b	129.7 (2)	0.135 (3)	2
134 K			
D_{a1}	179.5 (4)	0.130 (3)	1
D_{a2}	141.4 (3)	0.172 (3)	1
D_{b1}	167.1 (3)	0.165 (3)	1
D_{b2}	121.2 (2)	0.216 (3)	1
D_{b3}	142.6 (2)	0.148 (2)	1
D_{b4}	111.3 (2)	0.248 (2)	1

Table 31A-2-011. $NaD_3(SeO_3)_2$. Direction cosines of the principal axes of the deuteron quadrupole coupling tensors at the deuteron positions at 298 K and 134 K [69Sod]. $X_c \parallel a'$ axis; $Y_c \parallel b'$ axis; Z_c: perpendicular to the $a'b'$ plane (compare also Fig. 31A-1-001).

		X_c	Y_c	Z_c
298 K				
D_a	ϕ_{xx}	0.5863 (87)	0.3359 (77)	0.7372 (37)
	ϕ_{yy}	0.7246 (70)	−0.6243 (39)	−0.2918 (91)
	ϕ_{zz}	0.3623 (13)	0.7053 (10)	−0.6094 (14)
D_b	ϕ_{xx}	−0.5595 (86)	−0.4099 (50)	0.7204 (40)
	ϕ_{yy}	0.8130 (59)	−0.4406 (43)	0.3807 (78)
	ϕ_{zz}	0.1613 (12)	0.7987 (7)	0.5797 (10)
134 K				
D_{a1}	ϕ_{xx}	0.6092 (87)	0.3147 (77)	0.7279 (41)
	ϕ_{yy}	0.7122 (73)	−0.6209 (37)	−0.3276 (91)
	ϕ_{zz}	0.3488 (11)	0.7180 (8)	−0.6024 (11)
D_{a2}	ϕ_{xx}	0.6232 (67)	0.3361 (59)	0.7062 (33)
	ϕ_{yy}	0.7148 (58)	−0.6112 (30)	−0.3400 (69)
	ϕ_{zz}	0.3173 (12)	0.7166 (8)	−0.6211 (12)
D_{b1}	ϕ_{xx}	−0.3009 (72)	−0.4962 (31)	0.8144 (11)
	ϕ_{yy}	0.9252 (24)	−0.3588 (41)	0.1232 (63)
	ϕ_{zz}	0.2311 (10)	0.7906 (7)	0.5671 (10)
D_{b2}	ϕ_{xx}	−0.3119 (58)	−0.5263 (28)	0.7911 (10)
	ϕ_{yy}	0.9163 (20)	−0.3867 (36)	0.1041 (50)
	ϕ_{zz}	0.2512 (10)	0.7573 (8)	0.6028 (11)
D_{b3}	ϕ_{xx}	−0.8351 (43)	−0.2755 (39)	0.4760 (54)
	ϕ_{yy}	0.5485 (66)	−0.4827 (20)	0.6828 (40)
	ϕ_{zz}	0.0417 (10)	0.8313 (5)	0.5542 (8)
D_{b4}	ϕ_{xx}	−0.3679 (41)	−0.5156 (21)	0.7739 (9)
	ϕ_{yy}	0.9082 (17)	−0.3778 (25)	0.1801 (35)
	ϕ_{zz}	0.1996 (9)	0.7691 (6)	0.6072 (9)

Table 31A-2-012. $NaD_3(SeO_3)_2$. e^2qQ/h, η of ^{23}Na and the direction cosines of the principal axes of the quadrupole coupling tensor [69Sod]. In the column of Y_c, the signs correspond to the two equivalent sets of direction cosines of the principal axes. The unit cell refers to the a', b', c' axial system.

T [K]		e^2Qq/h [MHz]		η	
298	Na	1.19 (2)		0.09 (2)	
256	Na (1)	1.24 (1)		0.61 (2)	
	Na (2)	1.22 (1)		0.13 (1)	
			X_c	Y_c	Z_c
298	Na	ϕ_{xx}	0.270 (21)	∓0.182 (24)	0.945 (39)
		ϕ_{yy}	0.936 (35)	∓0.179 (25)	−0.302 (122)
		ϕ_{zz}	0.224 (7)	±0.967 (2)	0.122 (9)
256	Na (1)	ϕ_{xx}	−0.221 (16)	±0.073 (9)	0.973 (4)
		ϕ_{yy}	0.940 (4)	∓0.251 (6)	0.233 (17)
		ϕ_{zz}	0.261 (6)	±0.965 (2)	−0.013 (8)
	Na (2)	ϕ_{xx}	0.963 (11)	∓0.236 (7)	0.127 (73)
		ϕ_{yy}	−0.143 (71)	∓0.049 (18)	0.989 (9)
		ϕ_{zz}	0.227 (6)	±0.971 (1)	0.081 (6)

Table 31A-2-013. $NaD_3(SeO_3)_2$. Quadrupole coupling tensors and direction cosines with respect to the crystalline a', b' and c^* axes [78Kas]. $\boldsymbol{c^* = a' \times b'}$.

	$eQ\phi_{ii}/h$ [kHz]	Direction cosine with respect to		
		a'	b'	c^*
11.8 °C	1211.9	−0.1915	0.9780	−0.0828
Na	677.3	0.9790	0.1844	−0.0867
	534.6	0.0695	0.0976	0.9928
−79.5 °C	1307.9	−0.2715	0.9622	0.0196
Na (1)	1139.3	0.9369	0.2596	0.2341
	168.6	−0.2213	−0.0819	0.9720
Na (2)	1281.3	−0.2354	0.9707	−0.0477
	738.5	0.1691	0.0892	0.9816
	542.8	0.9571	0.2230	−0.1851

Table 31A-2-014. $NaD_3(SeO_3)_2$. e^2qQ/h, η of ^{23}Na and direction cosines of the largest principal axes with respect to the crystallographic a', b' and c^* axes [77Kaw]. $\boldsymbol{c^* = a' \times b'}$.

T [°C]	Site	e^2qQ/h kHz	η	Direction cosines with respect to		
				a'	b'	c^*
20	I, II	1207 (25)	+0.16 (5)	0.182	±0.981	0.068
−75	I	1309 (40)	+0.74 (8)	0.267	±0.960	−0.078
−75	II	1309 (40)	−0.16 (8)	0.254	±0.966	0.042

Table 31A-2-015. $NaH_3(SeO_3)_2$. e^2qQ/h, η of ^{23}Na under high pressure [76Ale]. $p = 7 \cdot 10^8$ Pa, $T = -90$ °C.

	$\frac{e^2qQ}{h}$ kHz	η	Phase
Na	1198	0.08	I
NaI	1311	0.13	IV
NaII	1340	0.04	
NaI	1299	0.33	II
NaII	1280	0.26	
NaIII	1245	0.22	
NaIV	1280	0.27	
NaI	1321	0.20	III
NaII	1342	0.68	