

**Table 31A-1-001.**  $\text{LiH}_3(\text{SeO}_3)_2$ . Crystal structure [72Tel]. Fractional coordinates at RT. For assignment of atomic numbers, see Fig. 31A-1-002, Fig. 31A-1-003.

Atoms	$x$	$y$	$z$
	$10^{-5}$		
Se (1)	23300	39507 (23)	08800
Se (2)	76690 (20)	10074 (21)	91095 (26)
O (1)	19252 (40)	22747 (32)	– 13341 (47)
O (2)	79816 (38)	27366 (31)	110145 (46)
O (3)	30176 (43)	29114 (33)	36189 (49)
O (4)	70944 (42)	20193 (35)	61072 (49)
O (5)	47888 (42)	47641 (32)	05452 (46)
O (6)	51917 (40)	02447 (29)	91695 (44)
Li	00241 (150)	24866 (146)	48066 (160)
H (1)	32880 (84)	14685 (64)	– 09938 (82)
H (2)	61997 (106)	38177 (71)	07074 (98)
H (3)	55051 (60)	23084 (52)	52793 (75)

**Table 31A-1-002.**  $\text{LiH}_3(\text{SeO}_3)_2$ . Crystal structure [72Tel]. Anisotropic temperature parameters.  $b_{ij}$  is defined by Eq. (b) in Introduction. For assignment of atomic numbers, see Fig. 31A-1-002, Fig. 31A-1-003.

Atoms	$b_{11}$	$b_{22}$	$b_{33}$	$b_{12}$	$b_{13}$	$b_{23}$
	$10^{-5}$					
Se (1)	562 (30)	479 (21)	793 (34)	083 (19)	118 (26)	033 (21)
Se (2)	478 (30)	418 (19)	915 (36)	– 018 (19)	070 (25)	027 (21)
O (1)	917 (43)	682 (30)	1015 (51)	– 014 (35)	060 (40)	– 195 (38)
O (2)	777 (44)	602 (29)	1221 (54)	013 (34)	065 (40)	– 206 (36)
O (3)	747 (42)	823 (35)	1017 (47)	062 (32)	146 (39)	260 (36)
O (4)	797 (46)	924 (38)	1093 (54)	– 053 (31)	161 (42)	266 (37)
O (5)	774 (44)	684 (35)	1646 (70)	– 119 (34)	373 (48)	117 (38)
O (6)	756 (43)	555 (31)	1621 (67)	– 131 (31)	392 (47)	– 17 (37)
Li	1207 (112)	921 (68)	1245 (138)	33 (62)	355 (96)	28 (78)
H (1)	1903 (104)	910 (55)	1833 (108)	– 153 (58)	350 (83)	– 139 (62)
H (2)	2771 (150)	1408 (88)	2187 (126)	– 1046 (99)	732 (111)	– 187 (86)
H (3)	1097 (85)	1270 (59)	1967 (114)	– 025 (53)	249 (73)	129 (65)

**Table 31A-1-003.**  $\text{LiH}_3(\text{SeO}_3)_2$ . Crystal structure [72Tel]. Interatomic distances and angles at RT. For assignment of atomic numbers, see Fig. 31A-1-002, Fig. 31A-1-003.

Distances	Å	Angles	deg	Angles	deg
Se (1)–O (1)	1.760 (3)	O (1)–Se (1)–O (3)	101.52 (15)	O (1)–Li–O (3)	90.22 (35)
–O (3)	1.653 (3)	O (1)–Se (1)–O (5)	100.29 (12)	O (1)–Li–O (4)	88.03 (33)
–O (5)	1.720 (3)	O (3)–Se (1)–O (5)	104.64 (12)	O (1)–Li–O (5)	86.84 (37)
–O (2)	2.903 (2)	Se (1)–O (1)–H (1)	111.97 (31)	O (1)–Li–O (6)	92.36 (41)
–O (4)	3.184 (3)	Se (1)–O (5)–H (2)	116.31 (35)	O (2)–Li–O (3)	92.43 (34)
–O (5)	3.086 (3)	Se (1)–O (3)–H (3)	128.23 (21)	O (2)–Li–O (4)	89.34 (35)
–Li	3.097 (9)	O (2)–Se (2)–O (4)	99.43 (15)	O (2)–Li–O (5)	91.90 (41)
Se (2)–O (2)	1.691 (3)	O (2)–Se (2)–O (6)	103.64 (13)	O (2)–Li–O (6)	88.83 (38)
–O (4)	1.765 (3)	O (4)–Se (2)–O (6)	102.55 (13)	O (3)–Li–O (5)	90.39 (41)
–O (6)	1.670 (3)	Se (2)–O (6)–H (1)	119.21 (24)	O (3)–Li–O (6)	91.36 (38)
–O (1)	2.913 (3)	Se (2)–O (2)–H (2)	117.74 (28)	O (4)–Li–O (5)	90.27 (38)
–O (3)	3.113 (3)	Se (2)–O (4)–H (3)	116.92 (30)	O (4)–Li–O (6)	87.95 (40)
–O (6)	2.955 (3)				
Li–O (1)	2.126 (9)				
–O (2)	2.127 (9)				
–O (3)	2.162 (9)				
–O (4)	2.163 (9)				
–O (5)	2.216 (12)				
–O (6)	2.187 (12)				

**Table 31A-1-004.**  $\text{LiH}_3(\text{SeO}_3)_2$ . Crystal structure [72Tel]. Hydrogen bond distances and angles at RT. For assignment of atomic numbers, see Fig. 31A-1-002, Fig. 31A-1-003.

X	H	Y	Distances			Angles
			X–H Å	H...Y Å	X...Y Å	X–H...Y deg
O (1)–H (1)...	O (6)		1.040 (6)	1.517 (6)	2.552 (3)	173.25 (43)
O (5)–H (2)...	O (2)		1.141 (7)	1.378 (7)	2.518 (3)	176.56 (54)
O (4)–H (3)...	O (3)		1.003 (4)	1.649 (5)	2.646 (4)	172.27 (40)

**Table 31A-1-005.**  $\text{LiH}_3(\text{SeO}_3)_2$ .  $d_{i\lambda}$ ,  $g_{i\lambda}$  at 25 °C [63Ber].

$d_{11}$	$d_{12}$	$d_{13}$	$d_{15}$	$d_{24}$	$d_{26}$	$d_{31}$	$d_{32}$	$d_{33}$	$d_{35}$
$10^{-12} \text{ C N}^{-1}$									
23.2	–22.3	–12.1	–46.6	–12.8	–14.6	–18.4	5.5	19.9	53.2
$g_{11}$	$g_{12}$	$g_{13}$	$g_{15}$	$g_{24}$	$g_{26}$	$g_{31}$	$g_{32}$	$g_{33}$	$g_{35}$
$\text{m}^2 \text{ C}^{-1}$									
0.078	–0.107	–0.0051	–0.0935	–0.113	–0.129	–0.0302	–0.0391	0.0734	0.152

**Table 31A-1-006.**  $\text{LiH}_3(\text{SeO}_3)_2$ .  $s_{\lambda\mu}$  at 25 °C [63Ber].

$s_{11}$	$s_{22}$	$s_{33}$	$s_{44} + 2s_{23}$	$s_{55} + 2s_{13}$	$s_{66} + 2s_{12}$	$s_{35} + s_{15}$
$10^{-11} \text{ m}^2 \text{ N}^{-1}$						
2.94	3.41	8.67	23.6	10.8	20.7	7.5

**Table 31A-1-007.**  $\text{LiD}_3(\text{SeO}_3)_2$ .  $e^2qQ/h$ ,  $\eta$  of  $^7\text{Li}$  and the direction cosines of the principal axes of the field-gradient tensors at RT [69Sod]. For  $X_c$ ,  $Y_c$  and  $Z_c$  axes, see Fig. 31A-1-001. Signs  $\pm$  in the column for the  $Y_c$  correspond to the two equivalent sets of direction of the principal axes.

$e^2qQ/h = 33.9 (3) \text{ kHz}$ , $\eta = 0.593 (13)$			
	$X_c$	$Y_c$	$Z_c$
$\phi_{xx}$	–0.6273 (61)	$\pm 0.0506 (133)$	0.7771 (54)
$\phi_{yy}$	–0.2874 (105)	$\pm 0.9124 (15)$	–0.2914 (100)
$\phi_{zz}$	0.7238 (42)	$\pm 0.4062 (38)$	0.5578 (59)

**Table 31A-1-008.**  $\text{LiD}_3(\text{SeO}_3)_2$ . Direction cosines of the principal axes of the electric field-gradient tensors at the positions of deuterons at RT [69Sod]. For  $X_c$ ,  $Y_c$  and  $Z_c$  axes, see Fig. 31A-1-001. For positions  $D_\alpha$ ,  $D_\beta$ ,  $D_\gamma$  see Fig. 31A-1-004.  $D_\alpha$ ,  $D_\beta$ ,  $D_\gamma$  are three kinds of observed spectra.

		$X_c$	$Y_c$	$Z_c$
$D_\alpha$	$\phi_{xx}$	0.6552 (14)	0.7516 (7)	0.0763 (108)
$(D_\alpha)$	$\phi_{yy}$	-0.1246 (72)	0.0079 (81)	0.9922 (8)
	$\phi_{zz}$	0.7451 (7)	-0.6596 (8)	0.0988 (12)
$D_\beta$	$\phi_{xx}$	0.3827 (139)	0.6631 (122)	0.6433 (209)
$(D_\beta)$	$\phi_{yy}$	-0.5349 (106)	-0.4087 (185)	0.7395 (179)
	$\phi_{zz}$	0.7533 (6)	-0.6271 (10)	0.1982 (14)
$D_\gamma$	$\phi_{xx}$	-0.4379 (30)	-0.4978 (210)	0.7486 (123)
$(D_\gamma)$	$\phi_{yy}$	-0.0606 (133)	0.8471 (116)	0.5279 (171)
	$\phi_{zz}$	0.8970 (6)	-0.1858 (36)	0.4012 (10)

**Table 31A-1-009.**  $\text{LiD}_3(\text{SeO}_3)_2$ . Deuteron  $e^2qQ/h$  and  $\eta$  at RT [69Sod]. Three kinds of spectra,  $D_\alpha$ ,  $D_\beta$ ,  $D_\gamma$  were observed. For assignment of atomic numbers, see Fig. 31A-1-004.

	$e^2Qq/h$ [kHz]	$\eta$	Assignment
$D_\alpha$	107.8(10)	0.172(9)	O(6)- $D_\alpha$ ...O'(1)
$D_\beta$	127.9(10)	0.154(6)	O(2)- $D_\beta$ ...O'(5)
$D_\gamma$	181.1(5)	0.101(4)	O(4)... $D_\gamma$ -O'(3)

**Table 31A-1-010.**  $\text{LiH}_3(\text{SeO}_3)_2$ .  $e^2qQ/h$ ,  $\eta$  and direction cosines for principal components of the electric field gradient tensor for  $^7\text{Li}$  at hydrostatic pressures  $1 \cdot 10^5$  Pa,  $3.3 \cdot 10^8$  Pa,  $5.9 \cdot 10^8$  Pa at RT [75Ser].  $X$ ,  $Y$ ,  $Z$ : Principal coordinates system.  $X \parallel a$ ,  $Y \parallel b$ ,  $Z \parallel c'$ . The  $\pm$  signs correspond to the two EFG tensors.

$\rho$	Quadrupole coupling constant and $\eta$	Direction cosines		
		$X$	$Y$	$Z$
$1 \cdot 10^5$ Pa	$\frac{e^2Qq}{h} = 35.64$ (100) kHz $\eta = 0.487$ (25)	$\phi_{xx} - 0.6674$	$\pm 0.0897$	$+0.7393$
		$\phi_{yy} \mp 0.2513$	$+0.9074$	$\mp 0.3369$
		$\phi_{zz} + 0.7010$	$\pm 0.4106$	$+0.5830$
$3.3 \cdot 10^8$ Pa	$\frac{e^2Qq}{h} = 35.23$ (100) kHz $\eta = 0.361$ (25)	$\phi_{xx} - 0.7110$	$\pm 0.2062$	$+0.6722$
		$\phi_{yy} \mp 0.1677$	$+0.8787$	$\mp 0.4469$
		$\phi_{zz} + 0.6829$	$\pm 0.4304$	$+0.5902$
$5.9 \cdot 10^8$ Pa	$\frac{e^2Qq}{h} = 34.63$ (100) kHz $\eta = 0.263$ (25)	$\phi_{xx} - 0.7465$	$\pm 0.3484$	$+0.5668$
		$\phi_{yy} \mp 0.0486$	$+0.8211$	$\mp 0.5687$
		$\phi_{zz} + 0.6636$	$\pm 0.4521$	$+0.5960$