Table 31A-7-001. $NH_4H_3(SeO_3)_2$. Crystal structure [72Tel]. Fractional coordinates [$\cdot 10^{-5}$] at RT.

	x	*y*	*z*
Se(1)	21 151(8)	39 349(3)	30 635(8)
Se(2)	75 695(9)	23 963(3)	17 355(8)
N	23 890(96)	08 216(27)	22 333(82)
O(1)	17 241(83)	42 222(23)	04 379(69)
O(2)	49 775(71)	22 250(24)	29 887(93)
O(3)	49 146(64)	42 744(21)	33 796(76)
O(4)	78 155(70)	33 322(21)	19 640(69)
O(5)	07 651(73)	45 911(22)	44 300(78)
O(6)	94 763(80)	20 530(24)	34 432(83)

Table 31A-7-002. $NH_4H_3(SeO_3)_2$. Crystal structure [72Tel]. Anisotropic temperature parameters b_{ij} [$\cdot 10^{-5}$] and root-mean-square displacements R_i [$\cdot 10^{-3}$ Å] along the principal axes. b_{ij} is defined by Eq. (b) in Introduction.

	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}	R_1	R_2	R_3
Se(1)	1 041(13)	99(1)	1 152(12)	–5(3)	–26(12)	–4(3)	126(1)	134(1)	153(1)
Se(2)	1 225(13)	140(2)	1 082(12)	–10(4)	49(13)	–17(3)	143(1)	146(1)	154(1)
N	1 517(131)	185(14)	1 471(108)	18(36)	204(122)	–33(34)	153(8)	172(7)	181(7)
O(1)	2 582(157)	223(14)	1 221(98)	–333(41)	–729(111)	147(31)	133(7)	151(7)	254(7)
O(2)	1 243(110)	246(14)	2 191(140)	–146(30)	42(129)	–106(40)	136(7)	193(7)	222(7)
O(3)	1 108(102)	172(12)	1 998(129)	32(27)	–67(104)	–109(34)	137(6)	159(7)	207(7)
O(4)	1 611(111)	130(10)	2 262(116)	–7(27)	225(139)	5(30)	144(6)	164(6)	216(6)
O(5)	1 392(105)	148(11)	2 106(123)	–4(31)	700(111)	–164(33)	122(8)	154(6)	228(6)
O(6)	1 729(119)	220(13)	2 159(145)	220(34)	–741(119)	–39(39)	130(7)	191(7)	236(7)

Table 31A-7-003. $NH_4H_3(SeO_3)_2$. Crystal structure [72Tel]. Interatomic distances [Å] and angles [°]. The first three digits of subscript code, the lattice translation (the asymmetric unit is in cell 555) and the fourth digits specifies the symmetry operation.

A. Distances [Å]		B. Angles [deg]	
Se(1)–O(1)	1.749(5)	O(1)–Se(1)–O(3)	97.42(26)
–O(3)	1.757(4)	O(1)–Se(1)–O(5)	103.05(22)
–O(5)	1.652(4)	O(3)–Se(1)–O(5)	98.27(21)
Se(2)–O(2)	1.737(5)	O(2)–Se(2)–O(4)	102.11(19)
–O(4)	1.676(4)	O(2)–Se(2)–O(6)	103.04(21)
–O(6)	1.667(5)	O(4)–Se(2)–O(6)	104.50(20)
O(1)H...$O(5)_{5642}$	2.648(6)	$O(1)_{5553}$–N–O(2)	71.61(17)
O(2)H...$O(6)_{4563}$	2.608(6)	$O(1)_{5553}$–N–$O(4)_{4553}$	57.66(15)
O(3)H...O(4)	2.546(6)	O(2) –N–$O(6)_{4551}$	67.58(15)
N–$O(1)_{5553}$	3.046(7)	$O(4)_{4553}$–N–$O(6)_{4551}$	84.48(17)
–O(2)	2.957(6)	$O(3)_{4563}$–N–$O(5)_{5454}$	89.17(17)
–$O(3)_{4563}$	3.129(8)	$O(3)_{4563}$–N–$O(5)_{5563}$	70.60(16)
–$O(3)_{6454}$	3.194(6)	$O(3)_{6454}$–N–$O(5)_{5454}$	68.86(14)
–$O(4)_{4553}$	3.056(7)	$O(3)_{6454}$–N–$O(5)_{5563}$	63.00(15)
–$O(5)_{5563}$	2.979(6)	$O(1)_{5553}$–N–$O(3)_{6454}$	59.99(15)
–$O(5)_{5454}$	3.048(6)	O(2) –N–$O(5)_{5563}$	75.78(16)
–$O(6)_{4551}$	2.877(6)	$O(4)_{4553}$–N–$O(5)_{5454}$	95.98(18)
		$O(6)_{4551}$–N–$O(3)_{4563}$	62.14(16)

$1 = x\,y\,z$; $2 = \frac{1}{2} - x, -y, \frac{1}{2} + z$; $3 = \frac{1}{2} + x, \frac{1}{2} - y, -z$; $4 = -x, \frac{1}{2} + y, \frac{1}{2} - z$.

Table 31A-7-004. $NH_4H_3(SeO_3)_2$. Crystal structure [76Gor]. Interatomic distances [Å] at –150 °C.

	–150 °C		–150 °C		–150 °C
Se 1–O 1	1.653 (4)	O 3···H–O′ 6	2.580 (4)	Se 1–Se′ 1	4.911 (3)
				Se 1–Se′ 2	3.807 (2)
Se 1–O 2	1.747 (5)	O 3–H···O 4	2.538 (5)	Se 1–Se″ 2	3.857 (1)
Se 1–O 3	1.750 (3)	O 1···H–O 2	2.611 (3)	Se 1–Se‴ 2	4.010 (2)
O 1–O 3	2.566 (4)	O 1–H 1	1.79	Se 1–Se⁗ 2	4.249 (3)
O 1–O 2	2.662 (5)	O 2–H 1	0.84	Se 1–O′ 1	3.664 (2)
O 2–O 3	2.624 (4)	O 5–H 2	1.71	Se 1–O′ 2	4.236 (1)
Se 2–O 4	1.669 (4)	O 6–H 2	0.85	Se 1–O 3	3.633 (1)
Se 2–O 5	1.680 (3)	O 3–H 3	1.04	Se 1–O′ 5	2.767 (3)
Se 2–O 6	1.747 (3)	O 4–H 3	1.56	Se 1–O 5	3.070 (4)
				Se 1–O″ 1	3.416 (2)
O 5–O 6	2.668 (6)	N–O 5	2.829 (6)		
O 5–O 4	2.640 (4)	N–O 4	2.916 (6)		
O 4–O 6	2.656 (5)	N–O 6	2.958 (5)		
		N–O 1	3.010 (4)		
		N–O 2	3.018 (5)		
		N–O′ 1	3.026 (6)		
		N–O 3	3.089 (5)		
		N–O′ 3	3.160 (4)		

Table 31A-7-005. $ND_4D_3(SeO_3)_2$, $RbD_3(SeO_3)_2$. Principal values and their direction cosines of the ^2D quadrupole coupling tensors with respect to the crystallographic ***a***, ***b***, ***c*** frame [81Vin]. α_z: angles between the q_{zz} directions of the two crystals, α_y: angles between the q_{yy} directions of the two crystals.

Hydrogen bonds	$ND_4D_3(SeO_3)_2$				$RbD_3(SeO_3)_2$			
	$eQ\phi_{ii}/h$ [kHz]	Direction cosines			$eQ\phi_{ii}/h$ [kHz]	Direction cosines		
		X	*Y*	*Z*		*X*	*Y*	*Z*
O(1)···O(5)	79.00	+0.0080	+0.9296	−0.3684	79.31	+0.0025	+0.9287	−0.3707
$\alpha_z = 1°$	93.50	−0.5322	+0.3158	+0.7855	90.19	−0.5198	+0.3179	+0.7929
$\alpha_y = 1.5°$	172.50	+0.8466	+0.1898	+0.4972	161.58	+0.8543	+0.1907	+0.4835
O(3)···O(4)	60.14	−0.6679	−0.0879	+0.7390	49.33	−0.5977	−0.2591	+0.7587
$\alpha_z = 3°$	85.38	−0.2651	+0.9559	−0.1258	72.70	−0.4175	+0.9084	−0.0187
$\alpha_y = 11°$	145.52	+0.6954	+0.2800	+0.6618	122.03	+0.6844	+0.3279	+0.6512
O(6)···O(2)	68.58	−0.4185	+0.1580	+0.8943	65.27	−0.5863	+0.2348	+0.7753
$\alpha_z = 5°$	87.46	+0.7794	−0.4430	+0.4430	83.42	+0.6309	−0.4679	+0.6188
$\alpha_y = 13°$	156.04	+0.4662	−0.8825	+0.0622	148.69	+0.5081	+0.8519	+0.1262