Table 31A-3-001. $KH_3(SeO_3)_2$. Crystal structure of phase I [69Han]. Fractional coordinates at RT. The crystallographic axes referred to are *a*, *b*, *c*.

Atoms	*x*	*y*	*z*
Se	0.15153 (4)	0.18806 (9)	0.21329 (9)
K	0.50000 (0)	0.18848 (32)	0.25000 (0)
O (1)	0.11114 (26)	0.38798 (67)	0.07151 (66)
O (2)	0.06727 (26)	0.11189 (70)	0.35833 (68)
O (3)	0.20691 (29)	0.32281 (75)	0.40645 (75)
H (1)	0.1830 (500)	0.4415 (1350)	0.4735 (1225)
H (2)	0.0135 (1000)	0.1164 (2600)	0.2700 (2700)

Table 31A-3-002. $KH_3(SeO_3)_2$. Crystal structure of phase I [69Han]. Bond angles.

Angles	deg
O (1)–Se–O (2)	100.61 (21)
O (1)–Se–O (3)	102.41 (21)
O (2)–Se–O (3)	99.82 (22)
Se–O (3)–H	111.96
Se–O (3)–H	119.34

Table 31A-3-003. $KH_3(SeO_3)_2$. Crystal structure of phase I [69Han]. Temperature parameters are defined by Eq. (d) in Introduction. The crystallographic axes referred to are *a*, *b*, *c*.

Atoms	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
	10^{-4} Å^2					
Se	161 (3)	243 (3)	239 (3)	23 (2)	10 (2)	8 (2)
K	256 (10)	284 (10)	246 (9)	0 (0)	48 (7)	0 (0)
O (1)	245 (24)	299 (23)	268 (21)	24 (19)	− 77 (18)	65 (17)
O (2)	225 (22)	390 (25)	235 (20)	−43 (19)	19 (17)	34 (18)
O (3)	243 (23)	429 (27)	366 (25)	16 (21)	−130 (20)	−118 (22)

Table 31A-3-004. $KD_3(SeO_3)_2$. Crystal structure of phase II [79Iwa]. Fractional coordinates by neutron diffraction method. The crystallographic axes referred to are *a*, *b*, *c*. $T = 80$ K.

	x	*y*	*z*
Se (1)	0.1498 (2)	0.1914 (7)	0.2149 (8)
Se (2)	0.3483 (2)	0.3187 (7)	0.7033 (7)
K	0.5005 (5)	0.1906 (19)	0.2321 (44)
O (1)	0.1096 (3)	0.3860 (10)	0.0685 (11)
O (2)	0.0694 (3)	0.0939 (10)	0.3615 (10)
O (3)	0.2110 (3)	0.3107 (9)	0.4093 (9)
O (4)	0.3891 (3)	0.1025 (9)	0.5733 (10)
O (5)	0.4341 (3)	0.3906 (11)	0.8615 (11)
O (6)	0.2949 (3)	0.1891 (12)	0.9058 (12)
D (1)	0.1763 (3)	0.4327 (13)	0.4690 (12)
D (2)	0.3312 (4)	0.0609 (11)	0.9667 (11)
D (3)	0.4871 (4)	0.3754 (12)	0.7373 (21)

Table 31A-3-005. $KD_3(SeO_3)_2$. Crystal structure of phase II [79Iwa]. Bond lengths [Å] and angles [°]. $T = 80$ K. Primed atoms are related to basis atoms by symmetry operation.

$DSeO_3$					
Se 1–O 1	1.669 (8)	O 1–O 2	2.695 (8)	O 1–Se 1–O 2	105.7 (4)°
Se 1–O 2	1.712 (7)	O 1–O 3	2.744 (8)	O 1–Se 1–O 3	108.0 (3)°
Se 1–O 3	1.723 (7)	O 2–O 3	2.670 (7)	O 2–Se 1–O 3	102.0 (3)°
De_2SeO_3					
Se 2–O 4	1.687 (7)	O 4–O 5	2.613 (9)	O 4–Se 2–O 5	98.7 (3)°
Se 2–O 5	1.757 (7)	O 4–O 6	2.627 (9)	O 4–Se 2–O 6	99.7 (4)°
Se 2–O 6	1.749 (8)	O 5–O 6	2.594 (8)	O 5–Se 2–O 6	95.4 (4)°
Hydrogen Bond					
D 1–O 3	1.007 (9)	D 2–O 6	1.068 (9)	D 3–O 5	1.160 (11)
D 1–O 4′	1.619 (9)	D 2–O 1′	1.594 (9)	D 3–O 2′	1.482 (9)
O 3–O 4′	2.612 (7)	O 6–O 1′	2.659 (9)	O 5–O 2′	2.600 (8)

Table 31A-3-006. $KD_3(SeO_3)_2$. The principal values and direction cosines of electric field gradient tensors of deuterons. Direction cosines at –53 °C are referred to the orthorhombic axes [78Kas]. See also [78Gra].

	$eQ\phi_{ii}/h$ kHz	Direction cosine with respect to		
		a	*b*	*c*
at 40.0 °C				
D (1)	151.4	0.5527	0.7349	−0.3930
	87.4	−0.2987	0.6149	0.7298
	64.0	−0.7780	0.2860	−0.5594
D (2)	129.0	0.8298	0.0	0.5580
	71.4	0.0	1.0000	0.0
	57.6	0.5580	0.0	−0.8298
at −53.0 °C				
D (1)	175.8	0.5503	0.7427	−0.3815
	100.5	−0.2719	0.5914	0.7591
	75.3	−0.7894	0.3140	−0.5274
D′ (1)	134.9	0.5490	0.7353	−0.3974
	79.8	−0.3512	0.6344	0.6886
	55.1	−0.7585	0.2384	−0.6065
D (2)	131.2	0.8234	−0.0564	0.5647
	75.2	−0.1321	0.9487	0.2874
	56.0	0.5519	0.3112	−0.7737

Table 31A-3-007. $KH_3(SeO_3)_2$. Chemical shift parameters of ^{77}Se nuclei [80Suk]. σ_{ii}: principal components of magnetic screening tensor.

T	Principal components relative to liquid H_2SeO_4		Direction cosines relative to crystallographic axes		
	[ppm]		*a*	*b*	*c*
−50 °C	σ_{xx}	−398	0.063	−0.216	0.974
($T > \Theta_{II-I}$)	σ_{yy}	−357	0.802	−0.570	−0.178
	σ_{zz}	− 54	0.594	0.793	0.138
−98 °C	$\sigma_{xx}(1)$	−415	0.054	−0.092	0.994
($T < \Theta_{II-I}$)	$\sigma_{yy}(1)$	−359	0.875	−0.475	−0.091
	$\sigma_{zz}(1)$	− 13	0.481	0.875	0.055
	$\sigma_{xx}(2)$	−383	0.345	−0.627	0.698
	$\sigma_{yy}(2)$	−351	0.590	0.434	0.681
	$\sigma_{zz}(2)$	− 81	0.730	0.647	0.220

Table 31A-3-008. $KH_3(SeO_3)_2:Cr^{3+}$. Spin Hamiltonian parameters at RT [78Zap]. A, B: two kinds of paramagnetic centers.

	g_x	g_y	g_z	D	E
				$\cdot 10^2\ m^{-1}$	
A	1.984	1.985	1.978	0.218	0.037
B	1.967	1.966	1.968	0.141	0.024

Table 31A-3-009. $KH_3(SeO_3)_2:VO^{2+}$. g and A tensors and the direction cosines of the principal axes with respect to the a, b and c axes [78Jai].

	Direction cosines with respect to		
	a	b	c
g tensor			
1.925 (1)	0.9683	0.0044	−0.2496
1.992 (2)	−0.0666	−0.9590	−0.2832
1.998 (2)	0.2406	−0.2832	0.9284
A tensor ($\cdot 10^{-2}\ m^{-1}$)			
174.8 (10)	0.9961	0.0878	0.0010
71.3 (20)	−0.0775	0.8739	0.4800
65.4 (20)	0.0412	−0.4782	0.8773

Table 31A-3-010. $KD_3(SeO_3)_2$. g and A tensors for one site of SeO_2^- [81Mac]. X-ray irradiated crystal. T = RT.

Eigenvalues	Direction cosines		
	a	b	c
$g_{xx} = 1.9984(3)$	0.124	0.694	0.709
$g_{yy} = 2.0300(3)$	0.289	0.659	−0.694
$g_{zz} = 2.0052(3)$	0.949	−0.291	0.119
$A_{xx} = 232(2) \cdot 10^2\ Am^{-1}$	0.119	0.685	0.719
$A_{yy} = 76(2) \cdot 10^2\ Am^{-1}$	0.250	0.682	−0.687
$A_{zz} = 85(2) \cdot 10^2\ Am^{-1}$	0.965	−0.242	0.067