Table 31A-5-001. $CsH_3(SeO_3)_2$. Crystal structure of phase I [78Cho]. Fractional coordinates [$\cdot 10^{-5}$] at RT. α[H(1)] = 0.68, α[H(6)] = 0.32, α: occupation number.

Atom	*x*	*y*	*z*
Cs	83 884(12)	23 298(16)	89 073(20)
Se(1)	21 390(7)	25 648(10)	59 247(12)
Se(2)	52 845(7)	24 999(10)	18 862(12)
O(1)	15 393(11)	26 063(16)	28 549(18)
O(2)	13 300(15)	2 888(18)	63 388(25)
O(3)	9 928(14)	42 605(19)	66 614(21)
O(4)	48 467(15)	1 545(15)	27 668(26)
O(5)	59 459(12)	38 031(16)	45 347(18)
O(6)	36 030(12)	34 863(17)	8 263(18)
H(1)	2 386(4)	2 904(6)	2 152(7)
H(2)	286(4)	95(11)	5 266(12)
H(3)	252(5)	4 826(10)	5 284(11)
H(4)	4 991(9)	130(13)	4 541(10)
H(5)	5 138(14)	4 728(13)	3 890(20)
H(6)	2 851(10)	3 040(14)	1 735(18)

Table 31A-5-002. $CsH_3(SeO_3)_2$. Crystal structure of phase I [78Cho]. Interatomic distances [Å] and angles [°] at RT. A prime indicates an atom outside the asymmetric unit.

Ionic bonds			
Cs – O (1)	3.223 (1)	Cs – O (4)	3.308 (2)
Cs – O (2)	3.281 (2)	Cs – O (5)	3.123 (2)
Cs – O (3)	3.270 (2)	Cs – O (6)	3.342 (2)
Cs – O (3)	3.278 (2)	Cs – H (1)	3.217 (4)
		Cs – H (6)	3.229 (9)
Covalent bonds			
O – Se – O	O – Se	Se – O	∠ O – Se – O
O (1) – Se (1) – O (2)	1.735 (1)	1.702 (1)	99.06 (7)
O (1) – Se (1) – O (3)	1.735 (1)	1.689 (1)	100.22 (6)
O (2) – Se (1) – O (3)	1.702 (1)	1.689 (1)	101.92 (7)
O (4) – Se (2) – O (5)	1.703 (1)	1.705 (1)	101.79 (7)
O (4) – Se (2) – O (6)	1.703 (1)	1.683 (1)	102.33 (7)
O (5) – Se (2) – O (6)	1.705 (1)	1.683 (1)	102.52 (6)
Hydrogen bonds			
O – H···O	O – H	H···O	O···O
O (1) – H (1)···O (6)	1.000 (4)	1.581 (4)	2.577 (1)
O (6) – H (6)···O (1)	1.028 (9)	1.558 (9)	2.577 (1)
O (2) – H (2)···O (2′)	1.013 (5)	1.563 (5)	2.576 (3)
O (3) – H (3)···O (3′)	1.000 (6)	1.543 (5)	2.539 (2)
O (4) – H (4)···O (4′)	1.011 (6)	1.558 (6)	2.566 (3)
O (5) – H (5)···O (5′)	1.040 (11)	1.511 (11)	2.529 (2)
Se – O – H···O – Se	∠Se – O – H	∠O – H···O	∠H···O – Se
Se (1) – O (1) – H (1)···O (6) – Se (2)	111.2 (2)	174.0 (4)	116.4 (2)
Se (1) – O (2) – H (2)···O (2′) – Se (1′)	112.0 (4)	177.7 (7)	114.3 (3)
Se (1) – O (3) – H (3)···O (3′) – Se (1′)	114.7 (3)	174.0 (5)	120.2 (2)
Se (2) – O (4) – H (4)···O (4′) – Se (2′)	112.0 (5)	173.8 (8)	118.1 (3)
Se (2) – O (5) – H (5)···O (5′) – Se (2′)	110.7 (6)	175.7 (10)	113.7 (5)
Se (2) – O (6) – H (6)···O (1) – Se (1)	113.1 (5)	170.8 (9)	111.7 (4)

Table 31A-5-003. $CsH_3(SeO_3)_2$. Frequencies and assignments of vibrational modes [66Kha]. Frequencies [$\cdot 10^2$ m^{-1}].

phase I (−120 °C)	phase II (−175 °C)	Assignment	phase I (−120 °C)	phase II (−175 °C)	Assignment
	275		850 vw	847	$\nu_1(O_2{}^*)SeO)$
310	308	ν'_4, ν''_4 $(O_2{}^*)SeO)$		873	
	323				
322	326	ν'_4 O*) SeO_2^-		967	
	335?		970	988	O−H···O
				992?	out-of-plane bend
360 vw[1])	358	ν''_4 O*) SeO_2^-		1025	
	371				
			1220	1225	
395	400	$\nu_2(O_2^*)$ SeO)	1270	1275	O−H···O
	417	ν_2(O*) SeO_2^-)	1300	1325	in-plane bend
417	437			1330?	
630 vw	630 vw (background)	$\nu'_3(O_2^*)$ SeO)	1600	1600	
			2250 vb[1])	2260 vb	
650	649	ν_1(O*) SeO_2^-)	2380	2390	O−H···O stretch
	663		2600	2630	combinations[2])
			2720 vb	2700	and overtones
685 vw	675	$\nu''_3(O_2^*)$ SeO)	2950 vb		
	693			3240	
755	755	ν_3(O*) SeO_2^-)	3400	3400	
	767				
825	817	ν''_3 (O*) SeO_2^-)			
	823				

*) Phase II has superlattice structure; length of the *c* axis is twice as big as that in phase I.

[1]) vw: very weak, vb: very broad.

[2]) Observed in the spectra of the polycrystalline film deposited on a BaF_2 substrate. In general, the frequencies observed in the spectra of the polycrystalline film are different from the corresponding frequencies in the mulled spectra.

Table 31A-5-004. $CsH_3(SeO_3)_2$. Tensors of the dipole-dipole interaction between nuclei Cs–Se in Cs^+–Se(2)O_3-fragment at 20 °C obtained from the angular dependence of the second moment of the Se(2) spectral line [82Kri]. For *X*, *Y*, *Z*, see caption of Table 31A-5-005.

Principal tensor values [Hz]				Direction cosines of the principal axes relative to the rectangular frame		
T_{kl}	D_{kl}	B_{kl}				
		$A=+83(17)$	$A=-83(17)$	*Z*	*X*	*Y*
21(17)	−112	+50(24)	+174(24)	−0.668	+0.744	+0.026
99(17)	+ 56	+50(24)	− 72(24)	−0.412	−0.400	+0.320
129(17)	+ 56	−10(24)	−102(24)	+0.620	+0.535	+0.571

Table 31A-5-005. $CsH_3(SeO_3)_2$. Parameters of the ^{77}Se chemical shift tensors [82Kri]. σ_{ii}: principal values of chemical shift tensor. The X axis is along the crystallographic a axis. The Y axis lies in the a–b plane forming a right angle with the a axis. The Z axis is orthogonal to the X and Y axes.

Phase	Principal components relative to liquid H_2SeO_4 [ppm]	Direction cosines of the principal tensor axes relative to the X, Y, Z axes			Isotropic average σ_{av} [ppm]	Shielding anisotropy $\Delta\sigma$ [ppm]	Asymmetry parameter η
		X	Y	Z			
Paraelectric	$\sigma_{xx}(1)$ −409	+0.032	−0.184	+0.983			
$T = 20\,°C$	$\sigma_{yy}(1)$ −300	−0.179	+0.966	+0.186	−271	249	0.66
	$\sigma_{zz}(1)$ −105	+0.983	+0.182	+0.002			
	$\sigma_{xx}(2)$ −351	+0.631	+0.228	+0.742			
	$\sigma_{yy}(2)$ −322	−0.152	+0.974	−0.170	−267	208	0.21
	$\sigma_{zz}(2)$ −128	+0.761	+0.006	−0.649			
Anti-	$\sigma_{xx}(1a)$ −430	+0.185	+0.315	+0.931			
ferroelectric	$\sigma_{yy}(1a)$ −343	+0.369	+0.855	−0.363	−242	433	0.30
$T = -150\,°C$	$\sigma_{zz}(1a)$ − 47	−0.911	−0.411	−0.042			
	$\sigma_{xx}(1b)$ −507	+0.423	−0.513	+0.747			
	$\sigma_{yy}(1b)$ −354	−0.459	+0.589	+0.665	−252	534	0.43
	$\sigma_{zz}(1b)$ −104	+0.781	+0.624	−0.013			
	$\sigma_{xx}(2a)$ −407	−0.150	+0.856	+0.494			
	$\sigma_{yy}(2a)$ −307	+0.676	+0.276	+0.437	−244	338	0.44
	$\sigma_{zz}(2a)$ − 19	+0.721	+0.437	−0.538			
	$\sigma_{xx}(2b)$ −371	+0.570	−0.356	+0.740			
	$\sigma_{yy}(2b)$ −340	+0.623	+0.774	−0.740	−255	301	0.15
	$\sigma_{zz}(2b)$ − 54	−0.535	+0.523	+0.663			

Table 31A-5-006. $CsH_3(SeO_3)_2$, $CsD_3(SeO_3)_2$. Principal values and their direction cosines of the ^{133}Cs quadrupole coupling tensors [81Vin]. For X, Y, Z, see caption of Table 31A-5-005.

	T [°C]	$eQ\phi_{ii}/h$ [kHz]	Direction cosines with respect to		
			X	Y	Z
$CsH_3(SeO_3)_2$	+ 18	308	+0.7169	−0.0006	+0.6971
		167	−0.1722	+0.9691	+0.1763
		141	−0.6755	−0.2464	+0.6949
	−101	325	+0.7234	−0.0306	+0.6897
		201	+0.2964	+0.9160	−0.2702
		124	−0.6235	+0.3999	+0.6717
Cs(1)	−144	375	+0.7128	+0.0535	+0.6993
		240	+0.3486	+0.8382	−0.4194
		135	−0.6086	+0.5427	+0.5788
Cs(2)	−144	284	+0.7176	−0.0438	+0.6951
		196	+0.0347	+0.9990	+0.0273
		88	−0.6959	+0.0047	+0.7184
$CsD_3(SeO_3)_2$	+ 18	313	+0.7110	−0.0470	+0.7010
		183	−0.3010	+0.8811	+0.3641
		130	−0.6348	−0.4705	+0.6120

Table 31A-5-007. $CsD_3(SeO_3)_2$. Principal values and their direction cosines of the ^2D quadrupole coupling tensors [81Vin]. For *X, Y, Z*, see caption of Table 31A-5-005.

	$eQ\phi_{ii}/h$ [kHz]	Direction cosines with respect to				$eQ\phi_{ii}/h$ HkHz]	Direction cosines with respect to		
		X	*Y*	*Z*			*X*	*Y*	*Z*
Paraelectric phase (+15 °C)					Antiferroelectric phase (−125 °C)				
D(1)	56.8	+0.6441	−0.1903	+0.7647	$D(1)_a$	50.9	+0.6006	+0.0602	+0.7972
	77.5	−0.1319	+0.9819	+0.1356		74.4	−0.2164	+0.9722	−0.0896
	134.3	+0.7535	+0.1882	−0.6299		125.4	+0.7696	+0.2264	−0.5969
D(2)	61.9	+0.0461	+0.9421	−0.3321	$D(1)_b$	46.2	+0.6101	+0.0347	+0.7915
	79.8	−0.3794	+0.3240	+0.8660		71.7	−0.1238	+0.9909	+0.0519
	141.7	+0.9241	+0.0861	+0.3724		117.9	+0.8726	+0.1297	−0.6089
D(3)	58.8	−0.4034	+0.5483	+0.7325	D(2)	67.6	+0.0274	+0.9658	−0.2578
	79.6	+0.6099	+0.7579	−0.2314		87.8	−0.3764	+0.2488	+0.8924
	138.4	+0.6821	−0.3534	+0.6402		155.5	+0.9260	+0.0726	+0.3704
D(4)	61.9	+0.2190	+0.9757	−0.0078	D(3)	64.8	+0.4216	−0.5732	−0.7026
	73.5	+0.9700	−0.2185	−0.1066		90.5	+0.6143	+0.7507	−0.2437
	135.5	+0.1057	−0.0157	+0.9942		155.3	+0.6670	−0.3288	+0.6686
D(5)	55.9	+0.6373	+0.3315	+0.6959	D(4)	67.5	+0.1928	+0.9806	−0.0348
	79.4	+0.2652	+0.7532	−0.6019		82.6	+0.9773	−0.1961	−0.0822
	135.4	+0.7235	−0.5681	−0.3922		150.2	+0.0874	+0.0182	−0.9960
					D(5)	65.2	+0.6510	+0.3889	+0.6518
						87.5	+0.2273	+0.7194	−0.6463
						152.7	+0.7242	−0.5755	−0.3799