Table 20A-3-001. SbSBr. Structure of phase I (T = 294 K) and phase III (T = 11 K) [85Inu]. Fractional coordinates and anisotropic temperature parameters. b_{ij} is defined by Eq. (b) in Introduction.

	x	y	z	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
Sb (294 K)	0.1211(2)	0.1323(1)	0.25	0.0042(2)	0.0033(1)	0.0274(9)	–0.0011(1)	0.0	0.0
Sb (11 K)	0.1235(1)	0.1321(1)	0.2777(7)	0.0001(1)	0.0007(1)	0.0002(6)	–0.0001(1)	0.0000(3)	0.0001(3)
S (294 K)	0.8389(5)	0.0473(4)	0.25	0.0030(5)	0.0019(3)	0.0183(24)	0.0004(3)	0.0	0.0
S (11 K)	0.8370(4)	0.0486(4)	0.2585(19)	0.0007(4)	0.0010(3)	0.0015(21)	0.0002(3)	–0.0008(14)	0.0012(11)
Br (294 K)	0.5134(2)	0.8239(2)	0.25	0.0055(3)	0.0023(2)	0.0268(12)	–0.0006(2)	0.0	0.0
Br (11 K)	0.5135(2)	0.8231(1)	0.25	0.0004(2)	0.0009(1)	–0.0005(9)	0.0000(1)	–0.0011(5)	–0.0002(4)

Table 20A-3-002. SbSBr Structure of phase I [86Sia]. Fractional coordinates and anisotropic temperature parameters [$\cdot 10^{-4}$ Å^2]. U_{ij} is defined by Eq. (d) in Introduction.

	x	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}
Sb	0.1210(3)	0.1323(2)	0.2500	215(11)	198(11)	178(10)	–42(8)
S	0.8381(9)	0.0477(8)	0.2500	186(31)	143(29)	102(27)	17(25)
Br	0.5135(5)	0.8230(4)	0.2500	294(17)	158(14)	159(14)	–40(12)

Table 20A-3-003. SbSBr. Structure of phase I [86Sia]. Interatomic distances [Å] and bond angles [°]. See Fig. 20A-3-001 for the numbers assigned to the atoms.

Sb– S(1)	2.473(8) Å	S(1)–Sb–S(2)	84.24(9)°
S(2)	2.671(5)	Br(1)	81.67(9)
S(3)	2.671(5)	Br(3)	145.25(7)
Sb–Br(1)	2.937(3)	S(2)–Br–S(3)	95.95(9)
Br(2)	2.937(3)	Br(3)	112.34(9)
Br(3)	3.633(4)	Br(4)	64.46(8)
Br(4)	3.633(4)	Br(2)	87.84(8)
		Br(1)	164.97(9)
S(1)–Br(1, 2)	3.555		
S(2)–Br(3)	3.459	Br(3)–Sb–Br(4)	66.19(6)
S(2)–Br(2)	3.895	Br(2)	127.28(8)
		Br(1)	82.42(8)
S(1)–S(2, 3)	3.453		
		Br(2)–Sb–Br(1)	84.97(9)
Br(1)–Br(2)	3.968		
Br(2)–Br(3)	4.360		

Table 20A-3-004. SbSBr. Pressure coefficients of Raman active modes at several temperatures [90Hoc].

$\omega(p = 1 \cdot 10^5$ Pa) [cm^{-1}]					ω_0 [cm^{-1}]				$1/\omega_0(\mathrm{d}\omega/\mathrm{d}p)_T$ [$\cdot 10^{-3}$ GPa^{-1}]				
T 295 K a)	295 K	70 K	37 K	25 K	295 K	70 K	37 K	25 K	295 K a)	295 K	70 K	37 K	25 K
43.5	44.0	43.0	43.0	43.0	44.7	43.3	43.7	43.6	159	133	157	123	147
–	–	–	–	59.0	58.2	55.5	62.1	57.2	–	–6.5	0	–14	–4
61.5	61.7	64.0	64.5	64.5	62.6	64.4	65.3	65.4	143	120	110	81	95
78.5	77.5	79.0	79.0	79.0	77.8	78.9	79.6	79.5	41	57	52	33	44
82.5	–	84.0	84.0	84.0	83.1	83.9	84.6	84.3	50	50	49	35	46
119.0	120.5	121.0	121.5	121.5	120.4	121.2	122.1	121.8	19	19	23	13	20
–	–	138.0	138.0	138.0	–	137.4	137.6	138.2	–	–	44	31	26
148.5	149.7	148.0	147.0	148.5	149.6	147.5	147.4	147.8	–12	–5.5	1	–1.6	–1
173.0	175.6	173.0	172.5	173.0	176.2	172.6	172.8	172.9	8	–1	15	11	14
232.5	233.7	235.0	235.5	235.0	234.5	235.5	236.4	236.1	25	30	33	26	31
264.0	–	–	–	–	257.5	–	–	–	16	32	–	–	–
266.0	267.5	266.8	264.0	264.0	267.7	265.1	266.6	263.4	20	bad fit	15	20	24
–	–	–	274.5	270.5	–	271.9	272.9	270.9	–	–	21	13	24
–	–	318.7	319.0	319.0	–	318.7	319.7	319.0	–	–	3	0	1.5
322.0	327.5	325.6	326.0	326.0	326.6	325.7	326.4	325.8	4.3	2	4.4	1.6	5
–	–	330.1	330.0	330.8	–	330.1	330.2	330.3	–	–	6	3.5	7

a) Values from [89Ten].

Table 20A-3-005. SbSBr, SbSI. NQR frequencies of ^{121}Sb and ^{123}Sb, asymmetry parameter η, and quadrupole coupling constant [69Pop]. Subscripts 121 and 123, on (e^2qQ/h) indicate that the quantities are for ^{121}Sb and ^{123}Sb, respectively.

Compound	T [°C]	ν [MHz]	Nucleus	Transition	η	$(e^2qQ/h)_{123}$ [MHz]	$(e^2qQ/h)_{121}$ [MHz]	$(e^2qQ/h)_{123}/(e^2qQ/h)_{121}$
SbSI	+ 60	ν_1 27.78	^{123}Sb	1/2 3/2				
	+ 60	ν_2 44.75	^{121}Sb	1/2 3/2				
	+ 60	ν_3 53.496	^{123}Sb	3/2 5/2	0.096(1)	376.4(5)	293.3(5)	1.274
	≈ 32	ν_4 80.77	^{123}Sb	5/2 7/2				
	≈ 32	ν_5 88.59	^{121}Sb	3/2 5/2				
	– 195	ν_1 36.966	^{123}Sb	1/2 3/2				
	– 195	ν_2 51.552	^{121}Sb	1/2 3/2				
	– 195	ν_3 54.507	^{123}Sb	3/2 5/2	0.311(2)	398.1(5)	312.4(5)	1.274
	– 195	ν_4 84.55	^{123}Sb	5/2 7/2				
	– 195	ν_5 92.10	^{121}Sb	3/2 5/2				
SbSBr	+ 30	ν_1 31.548	^{123}Sb	1/2 3/2				
	+ 30	ν_2 50.231	^{121}Sb	1/2 3/2	0.120(1)	420.2(5)	329.7(5)	1.274
	+ 30	ν_3 59.554	^{123}Sb	3/2 5/2				
	+ 30	ν_4 62.375	^{81}Br	1/2 3/2	–	–	–	–
	– 195	ν_1 32.509	^{123}Sb	1/2 3/2				
	– 195	ν_2 51.407	^{121}Sb	1/2 3/2	0.132(1)	428.9(5)	336.4(5)	1.275
	– 195	ν_4 60.695	^{123}Sb	3/2 5/2				
	– 195	ν_4 62.350	^{81}Br	1/2 3/2	–	–	–	–

Table 20A-3-006. SbSBr, SbSeBr, SbSI, SbSeI, SbTeI. Mössbauer parameters [75Don]. δ: isomer shift, eQV_{zz}: quadrupole coupling constant, Γ: line width, η: asymmetry parameter, A: maximum absorption effect. The values are with respect to $Ba^{121}SnO_3$ ($Ca^{121}SnO_3$ and $^{121}SnO_2$ for data quoted from [71Khi] and [72Ale], respectively). Probable experimental errors in present data are ±0.1 mm s^{-1} in δ, ±0.5 mm s^{-1} in eQV_{zz} and ±0.02 mm s^{-1} in Γ.

Compound	T [K]	δ [mm/s]	eQV_{zz} [K]	Γ [mm/s]	η	A [%]	Ref.
SbSBr	4.2	–14.9	10.4	2.9	0.14	4.9	75Don
SbSBr	77	–	11.2	–	0.139	–	72Sem
SbSBr	77	–14.6	–	5.2	–	–	71Khi
SbSBr	77	–15.5	–	4.5	–	–	72Ale
SbSeBr	4.2	–14.5	10.6	4.0	0	5.0	75Don
SbSeBr	77	–14.6	–	5.8	–	–	71Khi
SbSI	4.2	–14.8	12.3	3.0	0.31	9.5	75Don
SbSI	77	–15.1	10.3	3.0	0.31	4.6	75Don
SbSI	77	–	10.41	–	0.31	–	72Sem
SbSI	77	–15.2	–	4.3	–	–	71Khi
SbSI	77	–14.2	–	4.0	–	–	72Ale
SbSeI	4.2	–14.9	6.4	3.1	≈1	5.7	75Don
SbSeI	77	–17.4	–	4.1	–	–	72Ale
SbTeI	4.2	–14.0	–12.0	3.0	0.2	7.5	75Don
SbTeI	77	–14.7	–	3.5	–	–	72Ale