

**Table 20A-9-001.** SbSeI. Structure of phase I [82Vou]. Fractional coordinates.

	$x$	$y$	$z$
Sb	0.1185(1)	0.1281(1)	1/4
Se	0.8347(1)	0.0482(1)	1/4
I	0.5157(1)	0.82686(9)	1/4

**Table 20A-9-002.** SbSeI. Structure of phase I [82Vou]. Temperature parameters.  $U_{ij}$  [ $\cdot 10^{-4} \text{ \AA}^2$ ] is defined by Eq. (d) in Introduction.

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{12}$	$U_{23}$	$U_{13}$
Sb	169(5)	233(5)	259(5)	-34(3)	0	0
Se	122(5)	189(6)	198(6)	10(4)	0	0
I	218(5)	199(4)	222(5)	-31(3)	0	0

**Table 20A-9-003.** SbSeI. Structure of phase I [82Vou]. Interatomic distances [ $\text{\AA}$ ]. Numbers of atoms are given in Fig. 20A-9-001.

Sb–I(1)	3.150(1)	I(2)–I(3)	4.628(1)
–I(2)	3.150(1)	–Se(1)	3.791(1)
–I(3)	3.822(1)	–Se(2)	4.203(2)
–I(4)	3.822(1)		
–Se(1)	2.601(2)	I(3)–I(4)	4.145(0)
–Se(2)	2.796(1)	–Se(2)	3.602(1)
–Se(3)	2.796(1)		
		I(4)–Se(3)	3.602(1)
I(1)–I(2)	4.145(0)		
–I(4)	4.628(1)	Se(1)–Se(2)	3.680(1)
–Se(1)	3.791(1)	–Se(3)	3.680(1)
–Se(3)	4.203(2)	Se(2)–Se(3)	4.145(0)

**Table 20A-9-004.** SbSeI. Structure of phase I [82Vou]. Bond angles [°].

I(1)–Sb–I(2)	82.29(3)	Sb–I(1)–I(2)	48.85(2)
–I(3)	125.74(4)	–I(4)	54.99(2)
–I(4)	82.56(3)	–Se(1)	42.78(3)
–Se(1)	81.87(4)	–Se(3)	41.70(2)
–Se(2)	166.23(5)		
–Se(3)	89.76(3)	Sb–I(2)–I(3)	54.99(2)
		–Se(1)	42.78(3)
I(2)–Sb–I(3)	82.56(3)	–Se(2)	41.70(2)
–I(4)	125.74(4)		
–Se(1)	81.87(4)	Sb–I(3)–I(2)	42.45(2)
–Se(2)	89.76(3)	–I(4)	57.17(2)
–Se(3)	166.23(5)	–Se(2)	44.13(2)
I(3)–Sb–I(4)	65.67(2)	Sb–I(4)–I(1)	42.45(2)
–Se(1)	145.78(2)	–I(3)	57.17(2)
–Se(2)	63.74(3)	–Se(3)	44.13(2)
–Se(3)	111.19(4)		
		Sb–Se(1)–I(1)	55.35(3)
I(4)–Sb–Se(1)	145.78(2)	–I(2)	55.35(3)
–Se(2)	111.19(4)	–Se(2)	49.27(3)
–Se(3)	63.74(3)	–Se(3)	49.27(3)
Se(1)–Sb–Se(2)	85.91(4)	Sb–Se(2)–I(2)	48.54(3)
–Se(3)	85.91(4)	–I(3)	72.13(4)
		–Se(1)	44.82(3)
Se(2)–Sb–Se(3)	95.67(4)	–Se(3)	42.16(3)
		Sb–Se(3)–I(1)	48.54(3)
		–I(4)	72.13(4)
		–Se(1)	44.82(3)
		–Se(2)	42.16(3)