

**Table 20A-4-001.** BiSBr. Fractional coordinates of phase I [84Vou].

Atom		
Bi	<i>x</i>	0.1373(1)
	<i>y</i>	0.1306(0)
	<i>z</i>	1/4
S	<i>x</i>	0.8325(6)
	<i>y</i>	0.0522(5)
	<i>z</i>	1/4
Br	<i>x</i>	0.5114(3)
	<i>y</i>	0.8246(3)
	<i>z</i>	1/4

**Table 20A-4-002.** BiSBr. Temperature parameters of phase I [84Vou].  $U_{ij}$  [ $\text{\AA}^2$ ] is defined by Eq. (d) in Introduction.

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{12}$	$U_{23}$	$U_{13}$
Bi	0.0098(5)	0.0124(5)	0.0195(5)	−0.0027(2)	0	0
S	0.0076(18)	0.0108(19)	0.0215(25)	0.0008(15)	0	0
Br	0.0153(9)	0.0151(10)	0.0246(12)	−0.0021(7)	0	0

**Table 20A-4-003.** BiSBr. Interatomic distances of phase I [84Vou].

Atoms	Distances [ $\text{\AA}$ ]
Bi–S	2.607
	2.721
Bi–Br	3.038
	3.539
S–Br	3.450
	3.596
	3.990
S–S	3.556
	4.049
Br–Br	4.049
	4.340