No. 20A-4 BiSBr, Bismuth sulfide bromide

(M = 320.94)

1a Ferroelectric transition of BiSBr at –170 °C was found by Nitsche et al. in 1964. 64Nit

phase	II	I	
state	F [a])	P [a])	[a]) 64Nit
crystal system		orthorhombic [b])	[b]) 50Don
spacegroup		Pnam– D_{2h}^{16} [b])	
Θ [°C]	–170 [a])		

ρ = 6.5(7) · 10^3 kg m^{-3} at RT (ρ_X = 6.8(3) · 10^3 kg m^{-3}). 50Don
Color: dark red (needles). 60Nit

2a Synthesis: $Bi_2S_3 + BiBr_3 \rightarrow 3BiSBr$ (400 °C). 50Don
Mixtures of Bi, S and Br or of 2Bi, 3S and $BiBr_3$ or of Bi_2S_3 and $BiBr_3$ were reacted in sealed, evacuated glass ampoules (500…600 °C). 60Nit, 64Nit
c axis oriented polycrystals: BiSBr needles whose axes are all parallel to each other were obtained by means of Bridgman furnace. 64Nit
Single crystals: needle crystals were obtained by slowly cooling the molten compound. 60Nit
See also 69Pop

b Crystal form: needle-like along *c*. 84Vou

3a Unit cell parameters at RT: a = 8.1666(9) Å, b = 9.8532(9) Å, c = 4.0492 Å. 84Vou
See also 50Don

b Z = 4. 50Don
All atoms are at 4c positions of Pnam– D_{2h}^{16} in phase I.
Crystal structure: Fig. 20A-4-001.
Fractional coordinates: Table 20A-4-001.
Temperature parameters: Table 20A-4-002.
Interatomic distances: Table 20A-4-003; Fig. 20A-4-002.

5a Curie-Weiss constant: C = 1.5 · 10^5 K, Θ_p = 99 K, Θ_f = 108 K. 68Pik

b $\xi = -3 \cdot 10^8$ VC^{-3} m^5, $\zeta = 29 \cdot 10^9$ VC^{-5} m^9. 68Pik

c $P_s = 8.5 \cdot 10^{-2}$ C m^{-2}. 68Pik

10a Raman scattering: Fig. 20A-4-003.

11 Photoconductive properties, see 60Nit, 68Pik