No. 20A-3 SbSBr, Antimony sulfide bromide

(M = 233.71)

1a Ferroelectric transition of SbSBr at –180 °C was found by Nitsche et al. in 1964. 64Nit

b

phase	III	II	I	
state	F	F	P [a])	[a]) 64Nit
crystal system			orthorhombic [b])	[b]) 50Don
space group			Pnam– D_{2h}^{16} [b])	
Θ [°C]	–250.2 [c])		–180 [a])	[c]) 80Inu1

$\rho = 4.8(6) \cdot 10^3$ kg m^{-3}, ($\rho_X = 4.9(4) \cdot 10^3$ kg m^{-3}) at RT. 50Don
Color: orange (needles). 60Nit
Cleavage: crystals cleave along the needle axis (c axis).

2a Synthesis: $Sb_2S_3 + SbBr_3 \rightarrow 3SbSBr$. 50Don
Mixtures of Sb, S and Br, or of 2Sb, 3S and $SbBr_3$, or of Sb_2S_3 and $SrBr_3$ were reacted in sealed, evacuated glass ampoules. 60Nit, 64Nit
c axis oriented polycrystals: densely packed single-crystalline needles whose axes are all parallel to each other were obtained by using Bridgman furnace. 64Nit
Single crystals: needle crystals were obtained by slowly cooling the molten compound. 60Nit
Hydrothermal method: see 69Pop, 70Pop, 71Khi

3a Unit cell parameters: a = 8.2424(6) Å, b = 9.7556(4) Å, c = 3.9680(2) Å at RT. 86Sia
See also 50Don

b $Z = 4$. 50Don

All atoms are at 4c positions of Pnam – D_{2h}^{16} in phase I. 58Moo

Structure of phase I: Table 20A-3-001, Table 20A-3-002; Fig. 20A-3-001, Fig. 20A-3-002.
Structure at 295 K and 11 K: Fig. 20A-3-003.

5a Dielectric constant: Fig. 20A-3-004.
See also 80Inu1
Curie-Weiss constant: $C = 1.2 \cdot 10^5$ K, $\Theta_p = 80$ K. 68Pik
Effect of E_{bias} on Θ_f: $d\Theta_f/dE_{bias} \approx 1.1 \cdot 10^{-5}$ KV^{-1} m. 68Pik

b $\xi = -44 \cdot 10^8$ VC^{-3} m^5, $\zeta = 350 \cdot 10^9$ VC^{-5} m^9. 68Pik

c $P_s \approx 7.5 \cdot 10^{-2}$ C m^{-2} at RT. 68Pik
$P_s = 6.3 \cdot 10^{-2}$ C m^{-2} at 4.2 K. 80Inu2

6a Transition heat and transition entropy at Θ_{I-I} (= 91 K): $\Delta Q_m = 15.07$ Jmol^{-1}, $\Delta S_m = 0.17$ JK^{-1} mol^{-1}. 68Pik

9a Reflectivity spectra in glassy and crystalline states: Fig. 20A-3-005.
Birefringence near Θ_{III-II}: Fig. 20A-3-006.

b $n_a = 2.64$, $n_b = 3.13$, $n_c = 4.00$ at $\lambda = 570$ nm, see also 68Ohi

10a Raman scattering spectra at 300 K and 7 K: Fig. 20A-3-007.
Raman scattering spectra at high pressure: Fig. 20A-3-008, Fig. 20A-3-009.
Pressure derivatives of phonon frequency: Table 20A-3-004;
see also 89Ten

11	Conductivity: order of 10^{-7} Ω^{-1} m^{-1} at RT.	68Pik
	Photosensitivity: order of 10^{-8} Ω^{-1} m^2 W^{-1} (maximum at $\lambda \approx 550$ nm).	60Nit
	Band gap estimated from light absorption: $E_G \approx 2.2$ eV. $dE_G/dT \approx 9 \cdot 10^{-4}$ eV K^{-1}.	68Pik
	Band structure: see	86Suk
12	Magnetic susceptibility: see Fig. 20A-1-004.	
13a	NQR frequencies: Table 20A-3-005; Fig. 20A-3-010. Mössbauer spectrum: Table 20A-3-006; Fig. 20A-3-011.	
14	Temperature dependence of the (055) Bragg reflection: Fig. 20A-3-012.	