23 Ag_3AsS_3, Proustite family

23A Pure compounds

No. 23A-1 Ag_3AsS_3, Proustite

(M = 494.72)

1a A polar crystal structure was determined by Harker in 1936. Change of sign of the pyroelectric coefficient was reported by Gavilova et al. in 1978 when an external field was applied on the crystal. 36Har 78Gav

b

phase	IV	III	II **)	I *)
state	F			
crystal system	monoclinic [e])	trigonal [d])		trigonal [a])
space group	Cc– C_s^4 [e])	R3c– C_{3v}^6 [d])		R3c– C_{3v}^6 [a])
Θ [K]	≈25 [c])		≈50 [b])	≈60 [b])

[a]) 36Har
[b]) 83Bon
[c]) 73Bai
[d]) 86Kha
[e])85All

$\rho = 5.65 \cdot 10^3$ kg m^{-3}. 66Eng
Color: brilliant red. 36Har
*) Another phase transition (photoinduced phase transition) was reported around 210 K. 82Smo, 91Yan1, 92Xia
**) Incommensurately modulated structure. 84Kha1, 85Rya, 86Kha

See subsection 14a.

2a Crystal growth:
Stockbarger method: see 72Ark
Bridgman method (in closed quartz ampoules): see 71Dov

3a Unit cell parameters: a_h = 10.825(1) Å, c_h = 8.704(1) Å (hexagonal system) at RT, a_m = 8.388(1) Å, b_m = 10.707(1) Å, c_m = 8.678(1) Å, β_m = 131.78(1)° (monoclinic system) at 20K; $\boldsymbol{a}_m = (\boldsymbol{a}_h + 2\boldsymbol{b}_h + 2\boldsymbol{c}_h)/3$, $\boldsymbol{b}_m = \boldsymbol{a}_h$, $\boldsymbol{c}_m = -\boldsymbol{c}_h$. 85All
Unit cell parameters in phase III are three times of those in phase I. 86Kha

b Z = 6 at RT (in hexagonal cell). 85All
Crystal structure: Fig. 23A-1-001, Fig. 23A-1-002.
Structural parameters, atomic positions: see 36Har, 66Eng, 85All
Incommensurately modulated structure in phase II: see subsection 14a.
Effects of cooling rate on superstructural reflections: see 85Afo

4 Unit cell parameter c vs. T: see 78Abd, 86Kha

5a Dielectric constant: Fig. 23A-1-003; see also 75Nov, 78Gav
Dielectric constant in the incommensurate region: see 82Ale, 85Ale
Θ–p phase diagram: see subsection 13 below.

d	Pyroelectricity: see	75Nov, 78Gav
	Change of *c*-component of spontaneous polarization estimated from pyroelectric measurements: Fig. 23A-1-004.	
	Pyroelectric luminescence: see	88Bra
6a	Anomalies have been found on C_p vs. T curve at ≈ 27 K, 49.5(5) K and 60.5(5) K.	83Bon
8a	Elastic stiffness at 295 K: Table 23A-1-001.	
	For temperature dependence, see	82Smo
	Temperature dependence of sound velocity and sound attenuation: Fig. 23A-1-005; see also	81Vil, 82Bel, 86Bel
	Effect of illumination on sound attenuation around 210 K: Fig. 23A-1-006; see also	92Xia
b	Second harmonic acoustic waves: see	81Vil
9a	Refractive indices n_o and n_e at 20 °C: $n_o^2 = 7.483 + 0.474/(\lambda^2 - 0.09) - 0.0019\,\lambda^2$, $n_e^2 = 6.346 + 0.342/(\lambda^2 - 0.09) - 0.0011\,\lambda^2$ (λ: wave length in μm),	67Hul
	$n_o = 3.0190$, $n_e = 2.7391$ at $\lambda = 632.8$ nm; $n_o = 2.82$, $n_e = 2.58$ at $\lambda = 1150$ nm.	73Esy
	Infrared absorption: see	72Ark, 73Bye
	Reflection spectra and dielectric functions (κ', κ''): Fig. 23A-1-007, Fig. 23A-1-008.	
	Reflection spectra in the 2…30 eV photon range:	88Dov
	See also	88Spi
	Optically transparent in the wavelength of 0.6…13 μm.	67Hul
	Optical absorption: Fig. 23A-1-009, Fig. 23A-1-010, Fig. 23A-1-011, Fig. 23A-1-012; see also	91Yan1
	Optical absorption coefficient under isotropic compression: see	80Ger
c	Elastooptic constants: $p_{11} = 0.10$, $p_{12} = 0.19$, $p_{13} = 0.22$, $p_{31} = 0.24$, $p_{33} = 0.20$ at $\lambda = 632.8$ nm.	73Zub
e	SHG and nonlinear optical coefficient: see	67Hul, 83Adh
	Two-photon absorption: Fig. 23A-1-013.	
10a	Raman scattering: Fig. 23A-1-014; see also	83Reb, 72Ark, 73Bye, 79Smo, 83Ewe
b	Brillouin scattering: Fig. 23A-1-015, Fig. 23A-1-016; see also	82Smo
11	Dark conductivity: see	81Vil
	ac electric conductivity: Fig. 23A-1-017.	
	Activation energy for the electric conductivity: see	91Yan2
	Negative photoconductivity and photoinduced change in the dielectric constant: see	88Tay, 90Yan
	Effect of *p* on the electric conductivity: see	90Bab
	Photoluminescence (510 nm laser light excitation): see	91Gol
	X-ray photoelectron spectra: see	91Dov1
	Band structure (tight-binding method): see	91Dov2

13a	NMR of ^{109}Ag: see NQR of ^{75}As: Fig. 23A-1-018. Θ–p phase diagram determined by NQR study: Fig. 23A-1-019.	96Nor
14	Incommensurately modulated structure in phase II is 3$\boldsymbol{q}$–state, characterized by following six wavevectors in the hexagonal setting: $\boldsymbol{q}_1 = (1/3 - \delta_1, -(1/3 - \delta_1), 0, 1/3 - \delta_2)$, $\boldsymbol{q}_2 = -\boldsymbol{q}_1$, $\boldsymbol{q}_3 = (0, 1/3 - \delta_1, -(1/3 - \delta_1), 1/3 - \delta_2)$, $\boldsymbol{q}_4 = -\boldsymbol{q}_3$, $\boldsymbol{q}_5 = (-(1/3 - \delta_1), 0, 1/3 - \delta_1, 1/3 - \delta_2)$, $\boldsymbol{q}_6 = -\boldsymbol{q}_5$; $\delta_1 = 0.0063(3)$, $\delta_2 = 0.0125(3)$ at 57 K. X-ray diffraction due to structural modulation: Fig. 23A-1-020, Fig. 23A-1-021, Fig. 23A-1-022. Neutron diffraction in phase II: see See also	85Rya 84Nel 86Kha, 84Kha1, 84Kha2
b	X-ray diffuse scattering: see	89Afo
15	Domain structure was observed by optical method. Effects of mechanical load and of electric field were investigated.	85Gor
16	Etching of single crystals (in $FeCl_3$, KOH, HNO_3): see	72Ark