24 $Sn_2P_2S_6$ family

24A Pure compounds

No. 24A-1 $Sn_2P_2S_6$

(M = 491.68)

1a Ferroelectricity in $Sn_2P_2S_6$ was discovered by Carpentier and Nitsche in 1974. 74Car1

b

phase	II	I	
state	F [a])	P [a])	[a]) 74Car1
crystal system	monoclinic [b]) [d])	monoclinic [b]) [c])	[b]) 74Car2
space group	$P1n1-C_s^{2}$ [d]) *)	$P12_1/n1-C_{2h}^{5}$ [c]) *)	[c]) 92Sco
Θ [°C]	66(2) [a])		[d]) 74Dit

P_s || nearly [100] in the (010) plane. 74Car1
T_{melt} = 775 °C. 74Car2
$\rho = 3.54 \cdot 10^3$ kg m^{-3}, $\rho_X = 3.57 \cdot 10^3$ kg m^{-3} at RT. 74Dit
Transparent, yellowish-brown. 74Car2
*) There are equivalent expressions of the space groups: P1c1 for P1n1 and $P12_1/c1$ for $P12_1/n1$, with the unit cell vectors $\boldsymbol{a}_c$, $\boldsymbol{b}_c$, $\boldsymbol{c}_c$ for $\boldsymbol{a}_n$, $\boldsymbol{b}_n$, $\boldsymbol{c}_n$. They are related by $\boldsymbol{a}_n = \boldsymbol{a}_c + \boldsymbol{c}_c$, $\boldsymbol{b}_n = \boldsymbol{b}_c$, $\boldsymbol{c}_n = -\boldsymbol{a}_c$. 74Car2

2a Crystal growth: vapor transport with iodine. 74Car2
b Crystal form: Fig. 24A-1-001.

3a Unit cell parameters: a_n = 9.362(2) Å, b_n = 7.493(1) Å, c_n = 6.550(3) Å, β_n = 91.17(3)° at 110 °C (phase I). 92Sco
a_n = 9.378(5) Å, b_n = 7.488(5) Å, c_n = 6.513(5) Å, β_n = 91.15(5)° at RT (phase II). 74Dit
On the space group Pc for phase II, a_c = 6.529(2) Å, b_c = 7.485(2) Å, c_c = 11.317(3) Å, β_c = 124.11(3)° at RT. 74Car2
b Z = 2. 74Car2, 74Dit, 92Sco
Crystal structure of phase I: Table 24A-1-001, Table 24A-1-002; Fig. 24A-1-002.
Crystal structure of phase II: Table 24A-1-003; Fig. 24A-1-003.

4 Thermal expansion coefficient: Fig. 24A-1-004; see also Fig. 24B-3-003 in No. 24B-3.

5a Dielectric constant: Fig. 24A-1-005, Fig. 24A-1-006, Fig. 24A-1-007, Fig. 24A-1-008.
Effect of hydrostatic pressure on dielectric constant: Fig. 24A-1-009.
Phase diagram in regard to hydrostatic pressure: Fig. 24A-1-010.
Effect of uniaxial stress on $\Theta_{I-I'}$: Fig. 24A-1-011.
$d\Theta_{I-I'}/dp = -240$ KGPa^{-1}. 84Tya
c Spontaneous polarization: Fig. 24A-1-012.
$P_s = 14 \cdot 10^{-2}$ Cm^{-2}, $E_c = 7.5 \cdot 10^4$ Vm^{-1} at 20 °C. 74Car1
Coercive field: Fig. 24A-1-013.
d Pyroelectric coefficient: see 90Vys1

6a	Heat capacity: Fig. 24A-1-014. See also Fig. 24B-3-008 in No. 24B-3.	
	See also	94Vas
b	Thermal conductivity: Fig. 24A-1-015.	
7a	Piezoelectric constant: Fig. 24A-1-016.	
	Electromechanical coupling factor: Fig. 24A-1-017.	
8	Sound velocity and attenuation, second ultrasonic harmonic generation:	
	Fig. 24A-1-018, Fig. 24A-1-019, Fig. 24A-1-020, Fig. 24A-1-021.	
	See also	87Val
9a	Birefringence: Fig. 24A-1-022.	
	Infrared spectra: see	77Gur
	Absorption: Fig. 24A-1-023.	
	Reflection spectra and electronic band structure: see	91Vlo
10a	Raman scattering: Fig. 24A-1-024.	
	See also	78Vys
11	Electrical conductivity: see	77But
	Photoconductivity: see	77Gur
14b	Density of phonon states: see	94Vas
15a	Domain structure: Fig. 24A-1-025; see also	96Gra
b	Switching process in the domain structure: see	91Gra
16	Laser evaporation growth of thin film: see	82Luk