Table 24A-1-001. $Sn_2P_2S_6$. Crystal structure of phase I [92Sco]. Fractional coordinates and isotropic temperature parameters U [$\cdot 10^{-3}$ Å^2], based on $P2_1/n$ unit cell. U is defined as one-third of the trace of the orthogonalized U_{ij} tensor. T = 110 °C.

Atom	x	y	z	U
Sn	0.2431(1)	0.3692(1)	–0.0411(1)	56(1)
S(1)	0.2629(2)	0.4975(2)	0.3991(3)	31(1)
S(2)	–0.0328(2)	0.3090(2)	0.1772(3)	28(1)
S(3)	0.0570(2)	0.1976(2)	0.6558(3)	29(1)
P	0.0671(2)	0.3914(2)	0.4394(3)	23(1)

Table 24A-1-002. $Sn_2P_2S_6$. Crystal structure of phase I [92Sco]. Interatomic distances. Symmetry codes: (i) x, y, z; (ii) $-x, -y, -z$; (iii) $1/2 - x, 1/2 + y, 1/2 - z$; (iv) $-1/2 + x, -1/2 - y, -1/2 + z$.

Atoms	[Å]	Atoms	[°]
Sn–S(1)	3.042(2)	S(1)–Sn–S(2)	69.3(1)
Sn–S(2)	3.014(2)	S(1)–Sn–S(1*b*)	90.0(1)
Sn–S(1*b*)^{iii}	2.937(2)	S(1)–Sn–S(2*b*)	93.6(1)
Sn–S(2*b*)^{ii}	3.227(2)	S(1)–Sn–S(2*c*)	131.2(1)
Sn–S(2*c*)^{iv}	3.122(2)	S(1)–Sn–S(3*b*)	144.5(1)
Sn–S(3*b*)^{i}	2.914(2)	S(1)–Sn–S(3*c*)	86.8(1)
Sn–S(3*c*)^{iii}	3.191(2)	S(1)–Sn–S(3*d*)	67.5(1)
Sn–S(3*d*)^{iv}	3.225(2)	S(2)–Sn–S(1*b*)	71.9(1)
S(1)–P	2.021(2)	S(2)–Sn–S(2*b*)	73.6(1)
S(2)–P	2.035(3)	S(2)–Sn–S(2*c*)	143.7(1)
S(3)–P	2.033(2)	S(2)–Sn–S(3*b*)	75.2(1)
P–P(*a*)^{ii}	2.213(2)	S(2)–Sn–S(3*c*)	137.6(1)
		S(2)–Sn–S(3*d*)	124.7(1)
		S(1*b*)–Sn–S(2*b*)	141.4(1)
		S(1*b*)–Sn–S(2*c*)	78.0(1)
		S(1*b*)–Sn–S(3*b*)	77.7(1)
		S(1*b*)–Sn–S(3*c*)	145.0(1)
		S(1*b*)–Sn–S(3*d*)	75.3(1)
		S(2*b*)–Sn–S(2*c*)	124.7(1)
		S(2*b*)–Sn–S(3*b*)	77.2(1)
		S(2*b*)–Sn–S(3*c*)	73.6(1)
		S(2*b*)–Sn–S(3*d*)	140.7(1)
		S(2*c*)–Sn–S(3*b*)	79.1(1)
		S(2*c*)–Sn–S(3*c*)	78.1(1)
		S(2*c*)–Sn–S(3*d*)	63.7(1)
		S(3*b*)–Sn–S(3*c*)	121.9(1)
		S(3*b*)–Sn–S(3*d*)	137.5(1)
		S(3*c*)–Sn–S(3*d*)	71.4(1)

Table 24A-1-003. $Sn_2P_2S_6$. Crystal structure of phase II based on Pn unit cell [74Dit]. Relation of the fractional coordinates (x, y, z) and those of the phase I (x', y', z'): (x', y', z'), by $x \approx -x' + 3/4$, $y = -y' - 3/4$, $z \approx z' - 1/4$.

Atom	x	y	z
Sn(1)	0.5270(2)	0.3856(2)	0.7224(3)
Sn(2)	0.0279(2)	0.1245(2)	0.7870(2)
P(1)	0.6836(4)	0.8608(5)	0.8108(6)
P(2)	0.8174(4)	0.64447(6)	0.6908(6)
S(1)	0.4898(4)	0.7511(6)	0.8491(6)
S(2)	0.7788(4)	0.9462(6)	0.0750(6)
S(3)	0.6942(4)	0.0517(5)	0.5921(6)
S(4)	0.0149(4)	0.7437(6)	0.6497(7)
S(5)	0.7147(4)	0.5633(5)	0.4288(6)
S(6)	0.8050(4)	0.4480(6)	0.9025(6)