Table 24A-2-001. $Sn_2P_2Se_6$. Structure of phase I [88Vor]. Fractional coordinates and isotropic temperature parameters. B [Å^2] is defined by Eq. (e) in Introduction.

Atom	x	y	z	B
Sn	0.7158(2)	0.3749(2)	0.7540(1)	2.80(3)
P	0.3751(4)	0.1062(4)	0.4351(3)	0.38(5)
Se(1)	0.8787(2)	0.0075(2)	0.7693(1)	0.80(2)
Se(2)	0.3917(2)	0.8084(2)	0.0560(1)	0.71(2)
Se(3)	0.7862(2)	0.6979(2)	0.9585(1)	0.68(2)

Table 24A-2-002. $Sn_2P_2Se_6$. Structure of phase I [88Vor]. Interatomic distances and bond angles.

Atom	Interatomic distances and bond angles
Sn–Se	3.00 Å–3.31 Å
P–Se	2.18 Å–2.19 Å
P–P	2.22 Å
Se–Sn–Se	66.6°–80.9°
	121.6°–146.4°
Se–P–Se	109.2°–116.1°
Se–P–P	103.6°–106.4°