

$\text{Ag}_{9.7}\text{Tl}_3\text{Se}_{6.5}$  $hP40$  $(176) P6_3/m - h^6cb$ **Tl<sub>6</sub>Ag<sub>20-x</sub>Se<sub>13-y</sub>** [1]

Structural features: Infinite columns of base-linked  $\text{Se}(\text{Tl}_2\text{Ag}_4)\text{Ag}_3$  and  $\text{Se}(\text{Tl}_4\text{Ag}_2)\text{Ag}_3$  tricapped trigonal prisms (partial vacancies ignored) share atoms to form a 3D-framework with  $\text{AlB}_2$ -type columns (7 prisms in the dented triangular cross-section); additional Se in channels of hexagonal cross-section parallel to [001] (partial disorder).

Klepp K.O. (1987) [1]

 $\text{Ag}_{9.71}\text{Se}_{6.49}\text{Tl}_3$  $a = 1.5116$ ,  $c = 0.4406$  nm,  $c/a = 0.291$ ,  $V = 0.8719$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Ag1	6h	$m..$	0.0824	0.3261	$1/4$	0.95	cuboctahedron $\text{Se}_4\text{Ag}_5\text{Tl}_3$
Se2	6h	$m..$	0.1426	0.5252	$1/4$		tricapped trigonal prism $\text{Ag}_5\text{Tl}_4$
Ag3	6h	$m..$	0.1906	0.0835	$1/4$		12-vertex polyhedron $\text{Se}_5\text{Ag}_7$
Se4	6h	$m..$	0.2374	0.2865	$1/4$		tricapped trigonal prism $\text{Ag}_7\text{Tl}_2$
Tl5	6h	$m..$	0.473	0.1881	$1/4$	0.86	22-vertex polyhedron $\text{Se}_8\text{Ag}_{10}\text{Tl}_4$
Ag6	6h	$m..$	0.579	0.0225	$1/4$		cuboctahedron $\text{Se}_4\text{Ag}_4\text{Tl}_4$
Ag7	2c	$-6..$	$1/3$	$2/3$	$1/4$		tricapped trigonal prism $\text{Se}_3\text{Tl}_6$
Se8	2b	$-3..$	0	0	0	0.49	square prism (cube) $\text{Se}_2\text{Ag}_6$

Transformation from published data: origin shift 0 0  $1/2$ Experimental: single crystal, diffractometer, X-rays,  $R = 0.040$ 

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Klepp K.O. (1987), J. Less-Common Met. 128, 131-142.