

$\text{Ag}_{22}\text{Tl}_4\text{Te}_{14.9}$	$hP46$	$(174) P-6 - 1^3k^3j^3hg^2feba$
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$\text{Tl}_4\text{Ag}_{24-x}\text{Te}_{15-y}$ [1]

Le Roy J. et al. (1992) [1]

$\text{Ag}_{22}\text{Te}_{14.88}\text{Tl}_4$

$a = 1.1418$, $c = 0.922$ nm, $c/a = 0.807$, $V = 1.0410$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	6l	1	0.12557	0.27493	0.2259		
Te2	6l	1	0.41947	0.10573	0.2621		tricapped trigonal prism Ag_7Tl_2
Ag3	6l	1	0.42257	0.35253	0.229		pentagonal bipyramid Te_4Ag_3
Ag4	3k	$m..$	0.05967	0.39133	$\frac{1}{2}$	0.667	4-vertex polyhedron AgTe_3
Ag5	3k	$m..$	0.28567	0.14433	$\frac{1}{2}$	0.667	
Te6	3k	$m..$	0.30917	0.42203	$\frac{1}{2}$		tricapped trigonal prism Ag_7Tl_2
Ag7	3j	$m..$	0.06887	0.42053	0		pentagonal bipyramid Te_4Ag_3
Ag8	3j	$m..$	0.28567	0.15733	0		
Te9	3j	$m..$	0.32117	0.42513	0		tricapped trigonal prism Ag_7Tl_2
Tl10	2h	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.244		23-vertex polyhedron $\text{Te}_9\text{Ag}_{12}\text{Tl}_2$
Te11	2g	3..	0	0	0.147	0.38	
Te12	2g	3..	0	0	0.305	0.5	
Tl13	1f	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{2}$		23-vertex polyhedron $\text{Te}_9\text{Ag}_{12}\text{Tl}_2$
Tl14	1e	-6..	$\frac{2}{3}$	$\frac{1}{3}$	0		23-vertex polyhedron $\text{Ag}_{12}\text{Te}_9\text{Tl}_2$
Te15	1b	-6..	0	0	$\frac{1}{2}$	0.5	
Te16	1a	-6..	0	0	0	0.62	

Transformation from published data: $-x, -y, -z$; origin shift $\frac{1}{3} \frac{2}{3} 0$

Experimental: single crystal, diffractometer, X-rays, $R = 0.100$

Remarks: Short interatomic distances for partly occupied site(s). In [1] the z -coordinate of former Te(2) is misprinted as 0.5 instead of 0 (agreement with Wyckoff position 3j; checked on interatomic distances).

References: [1] Le Roy J., Moreau J.M., Brun G., Liautard B. (1992), J. Alloys Compd. 186, 249-254.