

$\text{Tl}_{0.02}\text{V}_3\text{S}_4$	<i>hP18</i>	(176) $P6_3/m - h^2ed$
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$\text{Tl}_{0.033}\text{V}_6\text{S}_8$ [1]

Structural features: Units of three face-linked VS_6 octahedra share edges to form a 3D-framework; Tl in channels of hexagonal cross-section parallel to [001] (partial disorder). Filled-up derivative of Nb_3Te_4 .

Bensch W. et al. (1992) [1]

$\text{S}_4\text{Tl}_{0.02}\text{V}_3$

$a = 0.9137$, $c = 0.33071$ nm, $c/a = 0.362$, $V = 0.2391$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
V1	6 <i>h</i>	<i>m</i> ..	0.1215	0.4874	$\frac{1}{4}$		octahedron S_6
S2	6 <i>h</i>	<i>m</i> ..	0.2971	0.3474	$\frac{1}{4}$		non-coplanar triangle V_3
Tl3	4 <i>e</i>	3..	0	0	0.133	0.008	
S4	2 <i>d</i>	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		trigonal prism V_6

Experimental: single crystal, diffractometer, X-rays, $wR = 0.018$, $T = 293$ K

Remarks: We derived approximate values for the refinable atom coordinates from interatomic distances. Short interatomic distances for partly occupied site(s). In table 2 of [1] the chemical formula is misprinted as $\text{Tl}_{0.003}\text{V}_6\text{S}_8$ instead of $\text{Tl}_{0.033}\text{V}_6\text{S}_8$; on page 199 the occupancy of former site Tl is misprinted as 0.084 instead of 0.0084.

References: [1] Bensch W., Koy J., Wesemann M. (1992), J. Alloys Compd. 178, 193-204.