$Tl_{0.39}V_3S_4$	*hP*16	(176) $P6_3/m - h^2da$

$Tl_{0.78}V_6S_8$ rt [1]; $Ba_{0.44}V_6S_8$ [4]
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 with maximum probability for trigonal coordination). Filled-up derivative of Nb_3Te_4.

Bensch W. et al. (1992) [1]
$S_4Tl_{0.39}V_3$
$a = 0.9204$, $c = 0.33058$ nm, $c/a = 0.359$, $V = 0.2425$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
V1	6*h*	*m*..	0.1209	0.4884	$^1/_4$		octahedron S_6
S2	6*h*	*m*..	0.2975	0.3484	$^1/_4$		4-vertex polyhedron V_4
S3	2*d*	-6..	$^2/_3$	$^1/_3$	$^1/_4$		trigonal prism V_6
Tl4	2*a*	-6..	0	0	$^1/_4$	0.39	colinear Tl_2

Experimental: single crystal, diffractometer, X-rays, R = 0.021, T = 293 K

Remarks: Phase stable at T > 150-160 K. We derived values for the refinable atom coordinates from interatomic distances. The authors state that Tl is delocalized along [001] with maximum probability at Wyckoff position 2*a*. Short interatomic distances for partly occupied site(s). Supersedes structure proposals in space group (173) $P6_3$ with Tl (maximum probability) in octahedral [2] or intermediate site [3]. In table 2 of [1] the chemical formula is misprinted as $Tl_{0.078}V_6S_8$ instead of $Tl_{0.78}V_6S_8$.

References: [1] Bensch W., Koy J., Wesemann M. (1992), J. Alloys Compd. 178, 193-204. [2] Polborn K., Bensch W., Amberger E. (1985), J. Less-Common Met. 105, L5-L7. [3] Vlasse M., Fournès L. (1976), Mater. Res. Bull. 11, 1527-1532. [4] Fuentes O., Wang H.H., Ward B.H., Zhang J., Proserpio D.M., Calvagna F., Check C.E., Lobring K.C., Zheng C. (2001), Chem. Mater. 13, 3051-3056.