$Tl_{0.33}TaSe_2$	*hP*4	(187) *P*-6*m*2 – hba

$Tl_{0.33}TaSe_2$ [1]; $InNbS_2$ [2]; $In_{0.5}NbSe_2$ [4]; $In_{0.67}TaS_2$ [3]; $Tl_{0.5}TaS_2$ [5]
Structural features: Directly superposed close-packed Se layers; Ta and Tl in trigonal prismatic voids (stacking sequence AbAβ). $TaSe_6$ trigonal prisms share edges to form infinite slabs; Tl in trigonal prismatic voids between the slabs. Ignoring vacancies, substitution derivative of WC.

Müller D. et al. (1974) [1]
$Se_2TaTl_{0.33}$
a = 0.3473, c = 0.8353 nm, c/a = 2.405, V = 0.0873 nm^3, Z = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Se1	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.1981		non-coplanar triangle Ta_3
Tl2	1*b*	-6*m*2	0	0	$^1/_2$	0.328	anticuboctahedron Se_6Tl_6
Ta3	1*a*	-6*m*2	0	0	0		trigonal prism Se_6

Transformation from published data: -*x*,-*y*,-*z*
Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.074

Remarks: Refinement of the site occupancies showed no significant deviation from unity except for site Tl2.

References: [1] Müller D., Poltmann F.E., Hahn H. (1974), Z. Anorg. Allg. Chem. 410, 129-137. [2] Eppinga R., Wiegers G.A. (1980), Physica B+C (Amsterdam) 99, 121-127. [3] Di Salvo F.J., Hull G.W. Jr., Schwartz L.H., Voorhoeve J.M., Waszczak J.V. (1973), J. Chem. Phys. 59, 1922-1929. [4] Kulikov L.M., Romaka L.P., Aksel'rud L.G., Semenov Kobzar A.A. (1989), Vses. Konf. Kristallokhim. Intermet. Soeden., 5th, L'vov 1989, Coll. Abstr. p. 29. [5] Schmidt V. (1971), thesis, Tübingen U., Germany.