$Tl_{0.38}Ti_3Se_4$	*hP*20	(176) $P6_3/m$ – h^2edb

$Tl_{0.76}Ti_6Se_8$ [1]
Structural features: Units of three face-linked $TiSe_6$ 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.

Boiler H., Klepp K. (1983) [1]
$Se_4Ti_3Tl_{0.38}$
a = 0.9882, c = 0.359 nm, c/a = 0.363, V = 0.3036 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ti1	6*h*	*m*..	0.1292	0.4881	$^1/_4$		octahedron Se_6
Se2	6*h*	*m*..	0.2985	0.3483	$^1/_4$		4-vertex polyhedron Ti_4
Tl3	4*e*	3..	0	0	0.162	0.13	
Se4	2*d*	-6..	$^2/_3$	$^1/_3$	$^1/_4$		trigonal prism Ti_6
Tl5	2*b*	-3..	0	0	0	0.12	

Transformation from published data: *y*,*x*,-*z*; origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.077

Remarks: Short interatomic distances for partly occupied site(s). The authors of [2] (coordinates not published) place Tl preferentially in Wyckoff position 2*b* for composition $Tl_{0.8}Ti_6Se_8$ and $Tl_{0.64}Ti_6Se_8$ but in Wyckoff position 4*e* for $Tl_{0.23}Ti_6Se_8$. In [1] the Wyckoff position of former Tl(2) is misprinted as 4*a* instead of 4*e*.

References: [1] Boiler H., Klepp K. (1983), Mater. Res. Bull. 18, 437-442. [2] Bensch W., Koy J. (1992), Mater. Res. Bull. 27, 731-740.