$LiTl_3[MoO_4]_2$	*hP*28	(186) $P6_3mc$ – $c^2b^6a^2$

$Tl_3Li(MoO_4)_2$ [1]
Structural features: MoO_4 and LiO_4 tetrahedra share vertices to form a 3D-framework; Tl in channels delimited by 6-rings parallel to [001] and other voids.

Colbeau Justin C. et al. (1997) [1]
$LiMo_2O_8Tl_3$
a = 0.60037, c = 1.58194 nm, c/a = 2.635, V = 0.4938 nm^3, Z = 2

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
O1	6*c*	.*m*.	0.1726	0.8274	0.3758		single atom Mo
O2	6*c*	.*m*.	0.493	0.507	0.1782		non-colinear MoLi
O3	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.0307		single atom Mo
Mo4	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.1395		tetrahedron O_4
Mo5	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.4108		tetrahedron O_4
O6	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.5215		colinear MoLi
Li7	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.6357		tetrahedron O_4
Tl8	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.8402		11-vertex polyhedron $O_{10}Li$
Tl9	2*a*	3*m*.	0	0	0.0		non-coplanar triangle O_3
Tl10	2*a*	3*m*.	0	0	0.2407		9-vertex polyhedron O_9

Transformation from published data: origin shift 0 0 0.2593
Experimental: powder, diffractometer, neutrons, R_p = 0.047, T = 298 K

Remarks: The structure was studied jointly on powder neutron and single-crystal X-ray diffraction data.

References: [1] Colbeau Justin C., Wallez G., Xuriguera A.M., Elfakir A., Jaulmes S., Quarton M. (1997), Eur. J. Solid State Inorg. Chem. 34, 1097-1106.