

TlLaO ₃	<i>hP10</i>	(186) $P6_3mc - b^3a^2$
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TlLaO₃ α [1]

Structural features: Close-packed Tl and La layers in hc stacking; O in octahedral and tetrahedral voids.

Jouini N. et al. (1977) [1]

LaO₃Tl

$a = 0.3909$, $c = 1.2365$ nm, $c/a = 3.163$, $V = 0.1636$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.07		non-coplanar triangle La ₃
O2	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.35		non-coplanar triangle Tl ₃
Tl3	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.755		octahedron O ₆
La4	2 <i>a</i>	3 <i>m.</i>	0	0	0.0		7-vertex polyhedron O ₇
O5	2 <i>a</i>	3 <i>m.</i>	0	0	0.2		tetrahedron Tl ₃ La

Experimental: polycrystalline sample, electron diffraction, R = 0.120

Remarks: The description in space group (173) $P6_3$ in [1] does not take into consideration all symmetry elements of the proposed structure.

References: [1] Jouini N., Verbaere A., Tournoux M. (1977), Rev. Chim. Miner. 14, 435-440.