

Rb₁₅Tl₂₇*hP42*(189) *P-62m* – ji⁴hgeda**Rb₁₅Tl₂₇** [1]

Structural features: Layers containing single Tl₁₁ units (pentacapped trigonal prism) alternate with layers where similar units share prism edges and capping atoms.

Dong Z.C., Corbett J.D. (1996) [1]

Rb₁₅Tl₂₇

$a = 1.03248$, $c = 1.7558$ nm, $c/a = 1.701$, $V = 1.6210$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Tl1	6j	<i>m</i> ..	0.2920	0.4639	0		icosahedron Tl ₉ Rb ₃
Tl2	6i	.. <i>m</i>	0.3801	0	0.1005		icosahedron Tl ₇ Rb ₅
Rb3	6i	.. <i>m</i>	0.388	0	0.3156		pseudo Frank-Kasper Tl ₈ Rb ₅
Tl4	6i	.. <i>m</i>	0.7145	0	0.4089		bicapped square antiprism Tl ₄ Rb ₆
Rb5	6i	.. <i>m</i>	0.73	0	0.1892		15-vertex Frank-Kasper Tl ₉ Rb ₆
Tl6	4h	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1566		icosahedron Tl ₆ Rb ₆
Tl7	3g	<i>m2m</i>	0.2123	0	$\frac{1}{2}$		icosahedron Tl ₈ Rb ₄
Tl8	2e	3.. <i>m</i>	0	0	0.3490		icosahedron Tl ₆ Rb ₆
Rb9	2d	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		15-vertex polyhedron Tl ₉ Rb ₆
Rb10	1a	-62 <i>m</i>	0	0	0		pseudo Frank-Kasper Tl ₁₂ Rb ₆

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, wR = 0.048, T = 296 K

Remarks: Probably identical to the phase called RbTl₂ in [2]. Refinement of the site occupancies showed no significant deviation from unity. In table 1 of [1] the Hermann-Mauguin symbol for the space group is misprinted as *P-6m* instead of *P-62m* (given elsewhere).

References: [1] Dong Z.C., Corbett J.D. (1996), Inorg. Chem. 35, 1444-1450. [2] Thümmel R., Klemm W. (1970), Z. Anorg. Allg. Chem. 376, 44-63.