

$\text{Rb}_3\text{LaCl}_6[\text{H}_2\text{O}]_2$ $hP72$ $(176) P6_3/m - i^4h^3fb$ **$\text{Rb}_3\text{LaCl}_6 \cdot 2\text{H}_2\text{O}$** [1]

Structural features: Units of three edge-linked $\text{La}(\text{Cl}_6[\text{OH}_2]_2)$ square antiprisms arranged in slabs; Rb and additional Cl between the slabs.

Reuter G. et al. (1995) [1]

 $\text{Cl}_6\text{H}_4\text{LaO}_2\text{Rb}_3$ $a = 1.2204$, $c = 1.6886$ nm, $c/a = 1.384$, $V = 2.1780$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH ₂)1	12i	1	0.073	0.3458	0.1165		single atom La
Cl2	12i	1	0.1806	0.143	0.1507		non-colinear La ₂
Cl3	12i	1	0.4442	0.1451	0.0017		octahedron (OH ₂) ₂ Rb ₄
Rb4	12i	1	0.4651	0.3719	0.122		square antiprism Cl ₇ (OH ₂)
La5	6h	$m..$	0.0491	0.2393	$\frac{1}{4}$		square antiprism (OH ₂) ₂ Cl ₆
Cl6	6h	$m..$	0.3003	0.4515	$\frac{1}{4}$		single atom La
Cl7	6h	$m..$	0.4513	0.1427	$\frac{1}{4}$		single atom La
Rb8	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1202		tricapped trigonal prism Cl ₆ (OH ₂) ₃
Rb9	2b	-3..	0	0	0		octahedron Cl ₆

Transformation from published data: $y, x, -z$; origin shift 0 0 $\frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.088$

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Reuter G., Roffe M., Frenzen G. (1995), Z. Anorg. Allg. Chem. 621, 630-634.