

La₃[VO₄]Cl₆***hP30*****(176) *P6₃/m – h⁴fd*****La₃(VO₄)Cl₆ [1]**

Structural features: La(Cl₆O₂)(ClO) bicapped square antiprisms share atoms to form a 3D-framework; V in tetrahedral voids (statistical occupation of two face-sharing tetrahedra).

Kämmerer H., Gruehn R. (1996) [1]

Cl₆La₃O₄V $a = 1.25346$, $c = 0.41331$ nm, $c/a = 0.33$, $V = 0.5624$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cl1	6 <i>h</i>	<i>m</i> ..	0.14922	0.25271	¹ / ₄		4-vertex polyhedron La ₃ O
O2	6 <i>h</i>	<i>m</i> ..	0.21265	0.52121	¹ / ₄		
La3	6 <i>h</i>	<i>m</i> ..	0.40731	0.28214	¹ / ₄		
Cl4	6 <i>h</i>	<i>m</i> ..	0.44484	0.06597	¹ / ₄		non-colinear O ₂
V5	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.1732	0.5	pentagonal pyramid La ₄ O ₂
O6	2 <i>d</i>	-6..	² / ₃	¹ / ₃	¹ / ₄		colinear V ₂

Transformation from published data: *y*,*x*,*-z*

Experimental: single crystal, diffractometer, X-rays, R = 0.014

Remarks: In table 4 of [1] the *z*-coordinates of former site V is misprinted as 0.32680 instead of 0.82680 (checked on interatomic distances).

References: [1] Kämmerer H., Gruehn R. (1996), J. Solid State Chem. 122, 81-86.