

$\text{H}_{0.5}\text{La}_{6.17}[\text{VO}_4]_3\text{Cl}_{10}$ $hP70$ $(176) P6_3/m - ih^9da$ **La_{12.33}V₆O₂₃(OH)Cl₂₀ [1]**

Structural features: Infinite columns of base-linked $\text{La}(\text{Cl}_4\text{O}_2)\text{Cl}_3$ and $\text{La}(\text{Cl}_2\text{O}_4)\text{Cl}_3$ tricapped trigonal prisms and VO_4 tetrahedra (statistical occupation of two face-sharing tetrahedra) share atoms to form a 3D-framework; additional La in channels parallel to $[001]$ (partial disorder).

Kämmerer H., Gruehn R. (1998) [1]

 $\text{Cl}_{10}\text{H}_{0.50}\text{La}_{6.17}\text{O}_{12}\text{V}_3$ $a = 1.78729$, $c = 0.40545$ nm, $c/a = 0.227$, $V = 1.1217$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
V1	12i	1	0.18818	0.46752	0.1819	0.5	
Cl2	6h	$m..$	0.00543	0.58122	$1/4$		pentagonal bipyramid La_4O_3
Cl3	6h	$m..$	0.08267	0.17591	$1/4$		single atom La
M4	6h	$m..$	0.1104	0.3609	$1/4$		
M5	6h	$m..$	0.1593	0.5429	$1/4$		
La6	6h	$m..$	0.28247	0.22919	$1/4$		non-colinear O_2
M7	6h	$m..$	0.2916	0.4948	$1/4$		
Cl8	6h	$m..$	0.32492	0.08575	$1/4$		trigonal bipyramid La_3O_2
M9	6h	$m..$	0.4671	0.2797	$1/4$		non-colinear V_2
La10	6h	$m..$	0.53208	0.14757	$1/4$		non-coplanar square O_4
Cl11	2d	$-6..$	$2/3$	$1/3$	$1/4$		coplanar triangle La_3
La12	2a	$-6..$	0	0	$1/4$	0.167	colinear La_2

 $\text{M4} = 0.958\text{O} + 0.042\text{OH}$; $\text{M5} = 0.958\text{O} + 0.042\text{OH}$; $\text{M7} = 0.958\text{O} + 0.042\text{OH}$; $\text{M9} = 0.958\text{O} + 0.042\text{OH}$ Transformation from published data: $y, x, -z$; origin shift $0\ 0\ 1/2$ Experimental: single crystal, diffractometer, X-rays, $R = 0.035$

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Kämmerer H., Gruehn R. (1998), Z. Anorg. Allg. Chem. 624, 1526-1532.