

Cu_{8.67}La₁₃V_{4.33}O₃₉

hP136

(176) $P6_3/m - i^6h^9fcba$ **La₃Cu₂VO₉** [1]

Structural features: Infinite layers of LaO₈ cubes share vertices to form a 3D-framework; Cu in square voids. Units of nine vertex-linked CuO₄ squares.

Griend D.A.V. et al. (2001) [1]

Cu_{8.61}La₁₃O₃₉V_{4.39} $a = 1.4447$, $c = 1.0686$ nm, $c/a = 0.740$, $V = 1.9315$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12i	1	0.1139	0.3668	0.0744		single atom Cu
La2	12i	1	0.1488	0.5368	0.0085		square prism (cube) O ₈
O3	12i	1	0.1797	0.1312	0.0824		
La4	12i	1	0.3034	0.0732	0.0005		square prism (cube) O ₈
O5	12i	1	0.4031	0.4378	0.0766		single atom Cu
O6	12i	1	0.4982	0.2169	0.1079		single atom V
Cu7	6h	<i>m</i> ..	0.1231	0.3515	¹ / ₄		non-coplanar triangle O ₃
V8	6h	<i>m</i> ..	0.134	0.145	¹ / ₄	0.13	
Cu9	6h	<i>m</i> ..	0.1562	0.1379	¹ / ₄	0.87	
O10	6h	<i>m</i> ..	0.1903	0.5641	¹ / ₄		single atom V
O11	6h	<i>m</i> ..	0.2362	0.3103	¹ / ₄		
O12	6h	<i>m</i> ..	0.3474	0.0582	¹ / ₄		non-collinear VCu
Cu13	6h	<i>m</i> ..	0.3941	0.4193	¹ / ₄		coplanar square O ₄
V14	6h	<i>m</i> ..	0.489	0.194	¹ / ₄		tetrahedron O ₄
O15	6h	<i>m</i> ..	0.5519	0.0991	¹ / ₄		non-collinear VCu
O16	4f	3..	¹ / ₃	² / ₃	0.0775		single atom V
V17	2c	-6..	¹ / ₃	² / ₃	¹ / ₄		trigonal bipyramid O ₅
La18	2b	-3..	0	0	0		square prism (cube) O ₈
O19	2a	-6..	0	0	¹ / ₄		

Transformation from published data: origin shift 0 0 ¹/₂Experimental: powder, diffractometer, neutrons, time-of-flight, R_p = 0.044

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Griend D.A.V., Malo S., Barry S.J., Dabbousch N.M., Poeppelmeier K.R., Dravid V.P. (2001), Solid State Sci. 3, 569-579.