

Na₇[NH₄]₃V₁₅ClO₃₆[H₂O]₃₀

hP92

(189) *P*-62*m* – 1²kji⁶hg²f³a**(NH₄)₃Na₇[V₁₅O₃₆Cl]·30H₂O [1]**

Structural features: V₁₅ClO₃₆ units (a central Cl atom surrounded by fifteen VO₅ square pyramids sharing edges and vertices) in a HgSn₉-type (simple hexagonal) arrangement.

Shao M. et al. (1990) [1]

ClH₇₂N₃Na₇O₆₆V₁₅*a* = 1.3111, *c* = 1.113 nm, *c/a* = 0.849, *V* = 1.6569 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>l</i>	1	0.1571	0.2673	0.1281		non-coplanar triangle V ₃
(OH ₂)2	12 <i>l</i>	1	0.2887	0.4951	0.25		single atom Na
(OH ₂)3	6 <i>k</i>	<i>m</i> ..	0.2188	0.4795	¹ / ₂		4-vertex polyhedron (OH ₂) ₂ Na(NH ₄)
(OH ₂)4	6 <i>j</i>	<i>m</i> ..	0.1749	0.5535	0		non-colinear Na ₂
O5	6 <i>i</i>	.. <i>m</i>	0.1203	0	0.2691		non-coplanar triangle V ₃
V6	6 <i>i</i>	.. <i>m</i>	0.2367	0	0.1491		square pyramid O ₅
O7	6 <i>i</i>	.. <i>m</i>	0.3327	0	0.2385		single atom V
(OH ₂)8	6 <i>i</i>	.. <i>m</i>	0.5238	0	0.3399		single atom Na
O9	6 <i>i</i>	.. <i>m</i>	0.7681	0	0.3607		single atom V
V10	6 <i>i</i>	.. <i>m</i>	0.8422	0	0.2454		square pyramid O ₅
Na11	4 <i>h</i>	3..	¹ / ₃	² / ₃	0.1443		octahedron (OH ₂) ₆
(NH ₄)12	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.2282	0	¹ / ₂		non-colinear O ₂
Na13	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.6348	0	¹ / ₂		octahedron (OH ₂) ₄ O ₂
O14	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.2935	0	0		non-colinear V ₂
O15	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.6245	0	0		single atom V
V16	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.7469	0	0		square pyramid O ₅
Cl17	1 <i>a</i>	-62 <i>m</i>	0	0	0		36-vertex polyhedron V ₁₅ O ₂₁

Transformation from published data: origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, wR = 0.034

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

References: [1] Shao M., Leng J., Pan Z., Zeng H., Tang Y. (1990), Gaodeng Xuexiao Huaxue Xuebao 11, 280-285.