

$\text{NaNb}_6(\text{Nb}_{0.5}\text{V}_{0.5})_3\text{O}_{14}$
hP48

(176) $P6_3/m - i^2hg f^2da$
Na(V_{3-x}Nb_x)Nb₆O₁₄ [1]

Structural features: Infinite slabs containing Nb₆O₁₂O₆ clusters (a Nb₆ octahedron surrounded by an O₁₂ cuboctahedron and an O₆ large octahedron) sharing O atoms are interconnected via common vertices with (Nb,V)O₅ trigonal bipyramids and units of two face-linked (V,Nb)O₆ octahedra ((V,Nb)₂ dumbbells) to form a 3D-framework.

Köhler J. et al. (1989) [1]

 $\text{NaNb}_{7.46}\text{O}_{14}\text{V}_{1.54}$
 $a = 0.6034, c = 1.8079 \text{ nm}, c/a = 2.996, V = 0.5701 \text{ nm}^3, Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.1638	0.328	0.1287		non-coplanar triangle VNb ₂
Nb2	12 <i>i</i>	1	0.3086	0.1542	0.0638		5-vertex polyhedron O ₅
O3	6 <i>h</i>	<i>m</i> ..	0.0219	0.5098	¹ / ₄		coplanar triangle NbV ₂
O4	6 <i>g</i>	-1	¹ / ₂	0	0		coplanar square Nb ₄
M5	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.1792		octahedron O ₆
O6	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.6355		tetrahedron Nb ₄
M7	2 <i>d</i>	-6..	² / ₃	¹ / ₃	¹ / ₄		trigonal bipyramid O ₅
Na8	2 <i>a</i>	-6..	0	0	¹ / ₄		anticuboctahedron O ₁₂

 $M5 = 0.67V + 0.33Nb; M7 = 0.80Nb + 0.20V$

Experimental: single crystal, diffractometer, X-rays, wR = 0.027

Remarks: Refinement considering f(Nb) for site M5 and f(V) for site M7 gave occ(M5) = 0.471(2), occ(M7) = 0.152(1); the authors set approximate Nb/V ratios. In [1] the number of formula units per cell Z is misprinted as 3 instead of 2.

References: [1] Köhler J., Miller G., Simon A. (1989), Z. Anorg. Allg. Chem. 568, 8-21.