

Nb₃NiS₆*hP*24(182) *P*6₃22 – ifdcba**Ni_{0.33}NbS₂** [1]

Structural features: Close-packed S layers in BBCC stacking; Nb in trigonal prismatic, Ni in octahedral voids (partial order). Infinite slabs of edge-linked NbS₆ trigonal prisms are interconnected via NiS₆ octahedra to form a 3D-framework. Partly disordered variant of Nb₃CoS₆.

Van Laar B. et al. (1971) [1]

Nb₃Ni_{0.98}S₆*a* = 0.57518, *c* = 1.18796 nm, *c/a* = 2.065, *V* = 0.3404 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	12 <i>i</i>	1	0.003	0.3363	0.1315		trigonal prism Ni ₃ Nb ₃
Nb2	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.002		trigonal prism S ₆
Ni3	2 <i>d</i>	3.2	¹ / ₃	² / ₃	³ / ₄	0.901	octahedron S ₆
Ni4	2 <i>c</i>	3.2	¹ / ₃	² / ₃	¹ / ₄	0.014	octahedron S ₆
Ni5	2 <i>b</i>	3.2	0	0	¹ / ₄	0.062	octahedron S ₆
Nb6	2 <i>a</i>	32.	0	0	0		trigonal prism S ₆

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

Experimental: powder, diffractometer, neutrons, T = 293 K

Remarks: On page 156 of [1] the *z*-coordinate of the second Me site is misprinted as 0 instead of ¹/₄ (from table II) and the corresponding Wyckoff position as 2*a* instead of 2*b*.

References: [1] Van Laar B., Rietveld H.M., Ijdo D.J.W. (1971), J. Solid State Chem. 3, 154-160.