

$\text{Nb}_2\text{Ni}_2\text{P}_3$	$hP28$	$(176) P6_3/m - h^4ca$
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**Ni<sub>6</sub>Nb<sub>6</sub>P<sub>9</sub>** [1]

Structural features:  $\text{PNb}_6$  trigonal prisms and  $\text{P}(\text{Nb}_4\text{Ni}_2)\text{Ni}$  monocapped trigonal prisms (split Ni site; non parallel prism axes) share atoms to form a 3D-framework; additional P in channels parallel to [001] (partial disorder). Units of three face-linked  $\text{NbP}_6$  octahedra share edges to form a 3D-framework with channels of hexagonal cross-section parallel to [001]; Ni in square pyramidal coordination (partial disorder).

Guérin R. et al. (1981) [1]

$\text{Nb}_2\text{Ni}_2\text{P}_3$

$a = 1.0023$ ,  $c = 0.3408$  nm,  $c/a = 0.34$ ,  $V = 0.2965$  nm<sup>3</sup>,  $Z = 3$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Ni1	$6h$	$m..$	0.0997	0.2154	$\frac{1}{4}$	0.5	
Ni2	$6h$	$m..$	0.1234	0.2605	$\frac{1}{4}$	0.5	
P3	$6h$	$m..$	0.3688	0.3042	$\frac{1}{4}$		
Nb4	$6h$	$m..$	0.4882	0.1342	$\frac{1}{4}$		
P5	$2c$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism $\text{Nb}_6$
P6	$2a$	$-6..$	0	0	$\frac{1}{4}$	0.5	trigonal bipyramid $\text{P}_2\text{Ni}_3$

Transformation from published data: origin shift 0 0  $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.044$

Remarks: Additional reflections could be indexed with a 9-fold supercell (new axes 3a,3a,c).

References: [1] Guérin R., Potel M., Sergent M. (1981), J. Less-Common Met. 78, 177-187.