

$\text{Y}_6\text{Ni}_{14.92}\text{P}_{10.18}$  $hP70$  $(176) P6_3/m - h^{11}cb$  **$\text{Y}_6\text{Ni}_{15-x}\text{P}_{10+y}$  [1]**

Structural features: Infinite columns of base-linked  $\text{PY}_6\text{Ni}_3$ ,  $\text{P}(\text{Y}_4\text{Ni}_2)\text{Ni}_3$  and  $\text{P}(\text{Y}_2\text{Ni}_4)\text{Ni}_3$  tricapped trigonal prisms share atoms to form a 3D-framework with  $\text{AlB}_2$ -type columns (13 prisms in the dented triangular cross-section); additional P (partial disorder; splitting of neighboring site) in channels of hexagonal cross-section parallel to  $[001]$ . Variant of  $(\text{La}_{0.5}\text{Ce}_{0.5})_6\text{Rh}_{15}\text{P}_{10.5}$ .

Stoyko S. et al. (2004) [1]

 $\text{Ni}_{14.92}\text{P}_{10.18}\text{Y}_6$  $a = 1.6447$ ,  $c = 0.37891$  nm,  $c/a = 0.230$ ,  $V = 0.8876$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Ni1	6h	$m..$	0.0139	0.5647	$\frac{1}{4}$		tetrahedron $\text{P}_4$
P2	6h	$m..$	0.0241	0.2121	$\frac{1}{4}$		
P3	6h	$m..$	0.0764	0.4652	$\frac{1}{4}$		tricapped trigonal prism $\text{Ni}_5\text{Y}_4$
Ni4	6h	$m..$	0.0867	0.0528	$\frac{1}{4}$	0.188	
Ni5	6h	$m..$	0.1477	0.0871	$\frac{1}{4}$	0.785	
Ni6	6h	$m..$	0.1796	0.2521	$\frac{1}{4}$		
Ni7	6h	$m..$	0.2288	0.5124	$\frac{1}{4}$		tricapped trigonal prism $\text{P}_3\text{Y}_6$
P8	6h	$m..$	0.2795	0.4105	$\frac{1}{4}$		tricapped trigonal prism $\text{Ni}_5\text{Y}_4$
Ni9	6h	$m..$	0.347	0.0392	$\frac{1}{4}$		tetrahedron $\text{P}_4$
Y10	6h	$m..$	0.3599	0.2335	$\frac{1}{4}$		
Y11	6h	$m..$	0.5611	0.1774	$\frac{1}{4}$		21-vertex polyhedron $\text{P}_7\text{Ni}_8\text{Y}_6$
P12	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism $\text{Ni}_3\text{Y}_6$
P13	2b	-3..	0	0	0	0.18	octahedron $\text{Ni}_6$

Experimental: single crystal, diffractometer, X-rays,  $R = 0.056$ 

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

References: [1] Stoyko S., Oryshchyn S., Babizhetskii V., Guérin R. (2004), J. Alloys Compd. 367, 156-161.