

Ho₁₀Ni₃₃P_{21.5}

hP136

(176) $P6_3/m - h^{22}ca$ **Ho₂₀Ni₆₆P₄₃** [1]

Structural features: Infinite columns of base-linked P(Ho₄Ni₂)Ni₃ and P(Ho₂Ni₄)Ni₃ tricapped trigonal prisms share atoms to form a 3D-framework with propeller-like columns (21 P-centered prisms in the cross-section); additional P in channels of hexagonal cross-section parallel to [001] (partial disorder, splitting of neighboring site).

Pivan J. et al. (1985) [1]

Ho₁₀Ni₃₃P_{21.50} $a = 2.3095$, $c = 0.3742$ nm, $c/a = 0.162$, $V = 1.7285$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	6h	m..	0.0399	0.5016	$\frac{1}{4}$	0.5	cuboctahedron P ₄ Ni ₅ Ho ₃
Ni2	6h	m..	0.0513	0.3365	$\frac{1}{4}$		tricapped trigonal prism P ₃ Ho ₆
Ni3	6h	m..	0.0778	0.0684	$\frac{1}{4}$		
Ni4	6h	m..	0.0788	0.1831	$\frac{1}{4}$	0.5	square pyramid Ni ₅
P5	6h	m..	0.0974	0.4452	$\frac{1}{4}$		
Ni6	6h	m..	0.0989	0.0872	$\frac{1}{4}$		tricapped trigonal prism Ni ₅ Ho ₄
P7	6h	m..	0.1197	0.2965	$\frac{1}{4}$		
P8	6h	m..	0.1573	0.0347	$\frac{1}{4}$		
Ni9	6h	m..	0.1613	0.6109	$\frac{1}{4}$		13-vertex polyhedron P ₅ Ni ₈
Ni10	6h	m..	0.2101	0.525	$\frac{1}{4}$		cuboctahedron P ₄ Ni ₅ Ho ₃
Ho11	6h	m..	0.22846	0.22099	$\frac{1}{4}$		16-vertex polyhedron P ₆ Ni ₁₀
Ni12	6h	m..	0.2353	0.3614	$\frac{1}{4}$		cuboctahedron P ₄ Ni ₄ Ho ₄
Ni13	6h	m..	0.2688	0.1106	$\frac{1}{4}$		cuboctahedron P ₄ Ni ₄ Ho ₄
P14	6h	m..	0.2724	0.474	$\frac{1}{4}$		tricapped trigonal prism Ni ₇ Ho ₂
P15	6h	m..	0.3314	0.0591	$\frac{1}{4}$		tricapped trigonal prism Ni ₅ Ho ₄
Ho16	6h	m..	0.38165	0.39587	$\frac{1}{4}$		22-vertex polyhedron P ₈ Ni ₁₀ Ho ₄
Ho17	6h	m..	0.40554	0.23966	$\frac{1}{4}$		22-vertex polyhedron P ₈ Ni ₁₀ Ho ₄
Ni18	6h	m..	0.4472	0.1318	$\frac{1}{4}$		cuboctahedron P ₄ Ni ₅ Ho ₃
P19	6h	m..	0.5013	0.0718	$\frac{1}{4}$		tricapped trigonal prism Ni ₇ Ho ₂
Ni20	6h	m..	0.5508	0.2505	$\frac{1}{4}$		cuboctahedron P ₄ Ni ₅ Ho ₃
Ni21	6h	m..	0.6137	0.1226	$\frac{1}{4}$		cuboctahedron P ₄ Ni ₆ Ho ₂
P22	6h	m..	0.6363	0.2283	$\frac{1}{4}$		tricapped trigonal prism Ni ₇ Ho ₂
Ho23	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		23-vertex polyhedron P ₉ Ni ₁₂ Ho ₂
P24	2a	-6..	0	0	$\frac{1}{4}$	0.5	

Experimental: single crystal, diffractometer, X-rays, R = 0.054

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

References: [1] Pivan J., Guérin R., Sergent M. (1985), Mater. Res. Bull. 20, 887-896.