

Hf(Hf _{0.45} Nb _{0.55}) ₉ Ni ₃ P ₅	<i>hP</i> 18	(189) <i>P</i> -62 <i>m</i> – kf ³ cb
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Hf₅Nb₅Ni₃P₅ [1]

Structural features: Infinite columns of base-linked PHf₆(NbNi₂) and PHf₆Nb₃ tricapped trigonal prisms share atoms to form a 3D-framework.

Kleinke H., Franzen H.F. (1997) [1]

Hf_{4.96}Nb_{5.04}Ni₃P₅

a = 0.9561, *c* = 0.35237 nm, *c/a* = 0.369, *V* = 0.2790 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	6 <i>k</i>	<i>m</i> ..	0.215	0.43	¹ / ₂		7-capped pentagonal prism P ₄ Ni ₂ Nb ₄ Hf ₇
Ni2	3 <i>f</i>	<i>m2m</i>	0.2276	0	0		tricapped trigonal prism P ₂ NbHf ₆
M3	3 <i>f</i>	<i>m2m</i>	0.4961	0	0		rhombic dodecahedron NiP ₃ Hf ₈ Nb ₂
P4	3 <i>f</i>	<i>m2m</i>	0.772	0	0		tricapped trigonal prism Ni ₂ NbHf ₆
P5	2 <i>c</i>	-6..	¹ / ₃	² / ₃	0		tricapped trigonal prism Hf ₆ Nb ₃
Hf6	1 <i>b</i>	-62 <i>m</i>	0	0	¹ / ₂		pseudo Frank-Kasper Ni ₆ P ₆ Hf ₈

M1 = 0.595Hf + 0.405Nb; M3 = 0.869Nb + 0.131Hf

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

Experimental: single crystal, diffractometer, X-rays, *R* = 0.045, *T* = 295 K

Remarks: Homogeneity range Hf_{*x*}Nb_{10-*x*}Ni₃P₅, 4 < *x* < 6. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions.

References: [1] Kleinke H., Franzen H.F. (1997), J. Am. Chem. Soc. 119, 12824-12830.