

Er₅Zr₃Ni₁₆As₁₂*hP*36(189) *P*-62*m* – k²jg²f³ca**Er₅Zr₃Ni₁₆As₁₂** [1]; Ce₅Zr₃Ni₁₅As₁₂ [1]

Structural features: Infinite columns of base-linked As(Er₂Ni₄)(ZrNi₂), As(Er₄Ni₂)Ni₃ and As(Er₂Zr₂Ni₂)Ni₃ tricapped trigonal prisms share atoms to form a 3D-framework (a framework of base- and edge-linked As(Er₂Zr₂Ni₂) prisms with 6-fold prism columns shifted by *c*/2 in channels). Ordering variant of Hf₂Co₄P₃, [Er₅Zr₃]Ni₁₆As₁₂.

Pivan J.Y. et al. (1990) [1]

As₁₂Er₅Ni₁₆Zr₃*a* = 1.2651, *c* = 0.382 nm, *c/a* = 0.302, *V* = 0.5295 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
As1	6 <i>k</i>	<i>m</i> ..	0.1727	0.4821	1/2		tricapped trigonal prism Ni ₅ Zr ₂ Er ₂
Ni2	6 <i>k</i>	<i>m</i> ..	0.3602	0.481	1/2		cuboctahedron As ₄ Ni ₃ Zr ₂ Er ₃
Ni3	6 <i>j</i>	<i>m</i> ..	0.1822	0.3734	0		cuboctahedron As ₄ Ni ₄ ZrEr ₃
Ni4	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.2755	0	1/2		cuboctahedron As ₄ Ni ₄ Zr ₂ Er ₂
Er5	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.8198	0	1/2		22-vertex polyhedron As ₈ Ni ₁₀ Er ₄
As6	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.1773	0	0		square pyramid Ni ₅
Zr7	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.4365	0	0		14-vertex polyhedron As ₆ Ni ₈
As8	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.6471	0	0		tricapped trigonal prism Ni ₆ ZrEr ₂
Er9	2 <i>c</i>	-6..	1/3	2/3	0		23-vertex polyhedron As ₉ Ni ₉ Zr ₃ Er ₂
Ni10	1 <i>a</i>	-62 <i>m</i>	0	0	0		tricapped trigonal prism As ₃ Er ₆

Experimental: powder, diffractometer, X-rays, R = 0.049

References: [1] Pivan J.Y., Guérin R., Peña O., Padiou J., El Ghadraoui E.H., Rafiq M. (1990), Eur. J. Solid State Inorg. Chem. 27, 617-631.