

Dy₁₂Ni₃₀As₂₁ [1]

Structural features: Infinite columns of base-linked AsDy₆Ni₃, As(Dy₄Ni₂)Ni₃ and As(Dy₂Ni₄)Ni₃ tricapped trigonal prisms share atoms to form a 3D-framework with AlB₂-type columns (13 prisms in the dented triangular section); additional As in channels of hexagonal cross-section parallel to [001] (partial disorder; splitting of neighboring site). Variant of (La_{0.5}Ce_{0.5})₆Rh₁₅P_{10.5}.

Jeitschko W. et al. (2001) [1]

As_{10.30}Dy₆Ni₁₅

$a = 1.6985$, $c = 0.3877$ nm, $c/a = 0.228$, $V = 0.9686$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ni1	6 <i>h</i>	<i>m</i> ..	0.0142	0.5646	¹ / ₄		tetrahedron As ₄
As2	6 <i>h</i>	<i>m</i> ..	0.0253	0.2134	¹ / ₄		monocapped trigonal prism Ni ₇
Ni3	6 <i>h</i>	<i>m</i> ..	0.0751	0.0483	¹ / ₄	0.24	
As4	6 <i>h</i>	<i>m</i> ..	0.0776	0.4659	¹ / ₄		square pyramid Ni ₅
Ni5	6 <i>h</i>	<i>m</i> ..	0.1473	0.0877	¹ / ₄	0.76	
Ni6	6 <i>h</i>	<i>m</i> ..	0.1806	0.2518	¹ / ₄		tetrahedron As ₄
Ni7	6 <i>h</i>	<i>m</i> ..	0.2293	0.5126	¹ / ₄		coplanar triangle As ₃
As8	6 <i>h</i>	<i>m</i> ..	0.2801	0.4114	¹ / ₄		square pyramid Ni ₅
Ni9	6 <i>h</i>	<i>m</i> ..	0.3474	0.0383	¹ / ₄		tetrahedron As ₄
Dy10	6 <i>h</i>	<i>m</i> ..	0.36077	0.23536	¹ / ₄		
Dy11	6 <i>h</i>	<i>m</i> ..	0.56128	0.1776	¹ / ₄		21-vertex polyhedron As ₇ Ni ₈ Dy ₆
As12	2 <i>c</i>	-6..	¹ / ₃	² / ₃	¹ / ₄		coplanar triangle Ni ₃
As13	2 <i>b</i>	-3..	0	0	0	0.25	
As14	2 <i>a</i>	-6..	0	0	¹ / ₄	0.05	

Experimental: single crystal, diffractometer, X-rays, $R = 0.053$

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

References: [1] Jeitschko W., Terbüchte L.J., Rodewald U.C. (2001), *Z. Anorg. Allg. Chem.* 627, 2673-2679.