

ErNi₃Ge₂ [1]

Structural features: Infinite columns of base-linked Ge(Er₄Ni₂)Ni₃, Ge(Er₂Ni₄)(ErNi₂), Ge(Er₂Ni₄)Ni₃ and GeNi₆Er₃ tricapped trigonal prisms share atoms to form a 3D-framework with CaCu₅-type (PrNi₂Al₃) columns (7 Er atoms in the hexagonal cross-section) and propeller-like columns.

Oleksyn O.Y., Bodak O.I. (1994) [1]

ErGe₂Ni₃

$a = 1.79662$, $c = 0.37941$ nm, $c/a = 0.211$, $V = 1.0606$ nm³, $Z = 12$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Er1	3 <i>k</i>	<i>m</i> ..	0.0088	0.5756	$\frac{1}{2}$		21-vertex polyhedron Ge ₇ Ni ₁₁ Er ₃
Ni2	3 <i>k</i>	<i>m</i> ..	0.0906	0.159	$\frac{1}{2}$		cuboctahedron Ge ₄ Ni ₅ Er ₃
Er3	3 <i>k</i>	<i>m</i> ..	0.0969	0.3366	$\frac{1}{2}$		21-vertex polyhedron Ge ₇ Ni ₁₁ Er ₃
Ge4	3 <i>k</i>	<i>m</i> ..	0.1405	0.5176	$\frac{1}{2}$		icosahedron Ni ₇ Er ₃ Ge ₂
Ge5	3 <i>k</i>	<i>m</i> ..	0.148	0.069	$\frac{1}{2}$		bicapped square antiprism Ni ₇ Er ₃
Ni6	3 <i>k</i>	<i>m</i> ..	0.2404	0.2725	$\frac{1}{2}$		16-vertex Frank-Kasper Ge ₆ Ni ₇ Er ₃
Ge7	3 <i>k</i>	<i>m</i> ..	0.2827	0.4804	$\frac{1}{2}$		trigonal prism Ni ₆
Er8	3 <i>k</i>	<i>m</i> ..	0.3345	0.1678	$\frac{1}{2}$		16-vertex polyhedron Ge ₆ Ni ₁₀
Ni9	3 <i>k</i>	<i>m</i> ..	0.4229	0.0487	$\frac{1}{2}$		16-vertex Frank-Kasper Ge ₆ Ni ₇ Er ₃
Ge10	3 <i>k</i>	<i>m</i> ..	0.5217	0.2772	$\frac{1}{2}$		trigonal prism Ni ₆
Ni11	3 <i>k</i>	<i>m</i> ..	0.5817	0.1831	$\frac{1}{2}$		cuboctahedron Ge ₄ Ni ₅ Er ₃
Ni12	3 <i>j</i>	<i>m</i> ..	0.0571	0.4509	0		cuboctahedron Ge ₄ Ni ₄ Er ₄
Ge13	3 <i>j</i>	<i>m</i> ..	0.1457	0.2482	0		bicapped square antiprism Ni ₇ Er ₂ Ge
Ni14	3 <i>j</i>	<i>m</i> ..	0.1759	0.6205	0		cuboctahedron Ge ₄ Ni ₄ Er ₄
Ni15	3 <i>j</i>	<i>m</i> ..	0.1918	0.0037	0		cuboctahedron Ge ₄ Ni ₃ Er ₅
Ni16	3 <i>j</i>	<i>m</i> ..	0.1962	0.1541	0		cuboctahedron Ge ₄ Ni ₅ Er ₃
Ni17	3 <i>j</i>	<i>m</i> ..	0.2168	0.497	0		cuboctahedron Ge ₄ Ni ₄ Er ₄
Ni18	3 <i>j</i>	<i>m</i> ..	0.2602	0.385	0		cuboctahedron Ge ₄ Ni ₄ Er ₄
Ge19	3 <i>j</i>	<i>m</i> ..	0.3272	0.2933	0		bicapped square antiprism Ni ₅ Er ₄ Ge
Ge20	3 <i>j</i>	<i>m</i> ..	0.3363	0.041	0		bicapped square antiprism Ni ₅ Er ₄ Ge
Ni21	3 <i>j</i>	<i>m</i> ..	0.465	0.1803	0		cuboctahedron Ge ₄ Ni ₅ Er ₃
Ni22	3 <i>j</i>	<i>m</i> ..	0.4747	0.3216	0		cuboctahedron Ge ₄ Ni ₃ Er ₅
Ge23	3 <i>j</i>	<i>m</i> ..	0.5241	0.0859	0		bicapped square antiprism Ni ₇ Er ₂ Ge
Er24	1 <i>e</i>	-6..	$\frac{2}{3}$	$\frac{1}{3}$	0		23-vertex polyhedron Ge ₉ Ni ₁₂ Er ₂
Er25	1 <i>d</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		pseudo Frank-Kasper Ge ₆ Ni ₁₂ Er ₂
Er26	1 <i>a</i>	-6..	0	0	0		23-vertex polyhedron Ge ₉ Ni ₁₂ Er ₂

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 $\frac{1}{2}$

Experimental: powder, diffractometer, X-rays, $R_B = 0.059$

Remarks: Space group (176) *P*6₃/*m* was tested and rejected; we recommend space group (175) *P*6/*m* be tested. In the abstract of [1] the number of formula units per cell *Z* is misprinted as 6 instead of 12.

References: [1] Oleksyn O.Y., Bodak O.I. (1994), J. Alloys Compd. 215, 45-49.