

ErNi₃Al₉ Structure:

A9BC3_hR26_155_3cdef_c_f-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/9G5F>

https://aflow.org/prototype-encyclopedia/A9BC3_hR26_155_3cdef_c_f-001

Prototype	Al ₉ ErNi ₃
AFLOW prototype label	A9BC3_hR26_155_3cdef_c_f-001
ICSD	105031
CCDC	1662930
Pearson symbol	hR26
Space group number	155
Space group symbol	<i>R</i> 32
AFLOW prototype command	<code>aflow --proto=A9BC3_hR26_155_3cdef_c_f-001</code> <code>--params=a, c/a, x₁, x₂, x₃, x₄, y₅, y₆, x₇, y₇, z₇, x₈, y₈, z₈</code>

Other compounds with this structure

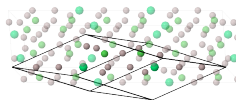
DyNi₃Al₉, ErNi₃Al₉, GdNi₃Al₉, YNi₃Al₉, YbNi₃Al₉, YbNi₃Ga₉

- DyNi₃Al₉ and YNi₃Al₉ have additional rare earth atoms on the (1b) (1/2 1/2 1/2) site and aluminum on another (6f) site, with partial occupancy on the rare earth (1b) and (1c) sites as well as the (3d) and both (6f) aluminum sites (Gladyshevskii, 1993, Table 2).
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

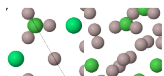
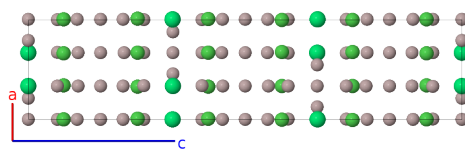
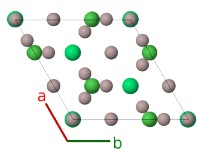
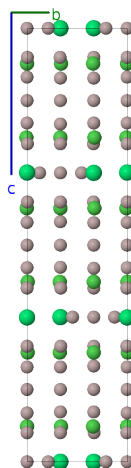
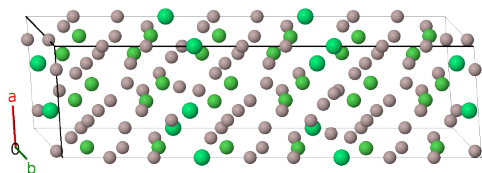
$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$





Basis vectors

Al
Er
Ni



	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$cx_1 \hat{\mathbf{z}}$	(2c)	Al I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-cx_1 \hat{\mathbf{z}}$	(2c)	Al I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(2c)	Al II
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-cx_2 \hat{\mathbf{z}}$	(2c)	Al II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$cx_3 \hat{\mathbf{z}}$	(2c)	Al III
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-cx_3 \hat{\mathbf{z}}$	(2c)	Al III
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$cx_4 \hat{\mathbf{z}}$	(2c)	Er I
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-cx_4 \hat{\mathbf{z}}$	(2c)	Er I
$\mathbf{B}_9$	$= y_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$\frac{1}{2}ay_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}}$	(3d)	Al IV
$\mathbf{B}_{10}$	$= -y_5 \mathbf{a}_1 + y_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}}$	(3d)	Al IV
$\mathbf{B}_{11}$	$= y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$	$=$	$\frac{1}{2}ay_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}}$	(3d)	Al IV
$\mathbf{B}_{12}$	$= \frac{1}{2} \mathbf{a}_1 + y_6 \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$\frac{1}{4}a(2y_6 + 1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a(6y_6 - 1) \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3e)	Al V
$\mathbf{B}_{13}$	$= -y_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3e)	Al V
$\mathbf{B}_{14}$	$= y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a(2y_6 - 1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a(6y_6 + 1) \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3e)	Al V
$\mathbf{B}_{15}$	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(6f)	Al VI
$\mathbf{B}_{16}$	$= z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + y_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(6f)	Al VI
$\mathbf{B}_{17}$	$= y_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(6f)	Al VI
$\mathbf{B}_{18}$	$= -z_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} - \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(6f)	Al VI
$\mathbf{B}_{19}$	$= -y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} - \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(6f)	Al VI
$\mathbf{B}_{20}$	$= -x_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 - y_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} - \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(6f)	Al VI
$\mathbf{B}_{21}$	$= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_8 - z_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_8 - 2y_8 + z_8) \hat{\mathbf{y}} + \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}}$	(6f)	Ni I
$\mathbf{B}_{22}$	$= z_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + y_8 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_8 - z_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_8 - y_8 - z_8) \hat{\mathbf{y}} + \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}}$	(6f)	Ni I
$\mathbf{B}_{23}$	$= y_8 \mathbf{a}_1 + z_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_8 - y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_8 + y_8 - 2z_8) \hat{\mathbf{y}} + \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}}$	(6f)	Ni I
$\mathbf{B}_{24}$	$= -z_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - x_8 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_8 - z_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_8 - 2y_8 + z_8) \hat{\mathbf{y}} - \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}}$	(6f)	Ni I
$\mathbf{B}_{25}$	$= -y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_8 - z_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_8 - y_8 - z_8) \hat{\mathbf{y}} - \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}}$	(6f)	Ni I
$\mathbf{B}_{26}$	$= -x_8 \mathbf{a}_1 - z_8 \mathbf{a}_2 - y_8 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_8 - y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_8 + y_8 - 2z_8) \hat{\mathbf{y}} - \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}}$	(6f)	Ni I

References

- [1] R. E. Gladyshevskii, K. Cenzual, H. D. Flack, and E. Parthé, *Structure of $R\text{Ni}_3\text{Al}_9$ ($R = \text{Y, Gd, Dy, Er}$) with either ordered or partly disordered arrangement of Al-atom triangles and rare-earth-metal atoms*, Acta Crystallogr. Sect. B **39**, 468–474 (1993), doi:10.1107/S010876819201173X.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.