$ErNi_3Al_9$ Structure: A9BC3_hR26_155_3cdef_c_f-001

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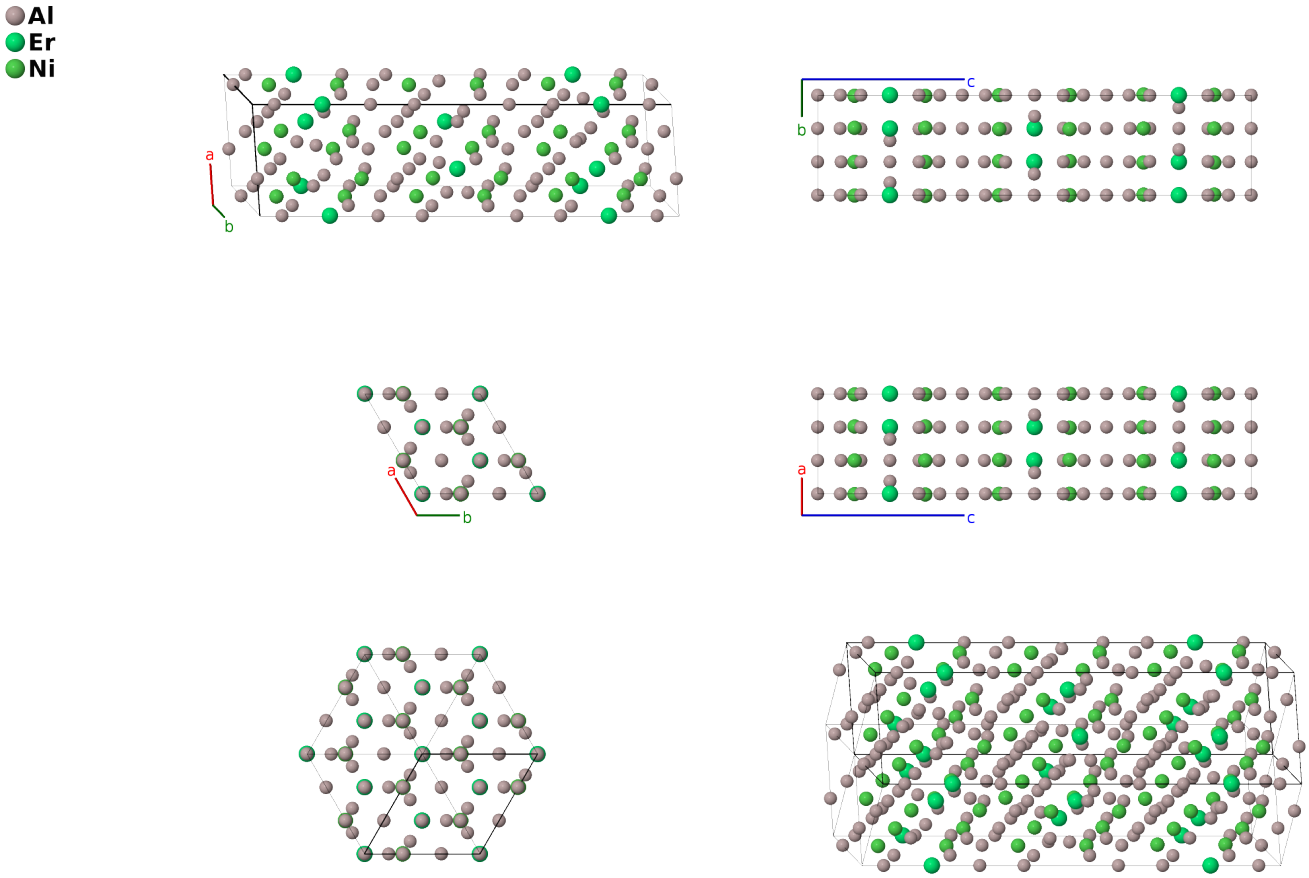
https://aflow.org/p/9G5F

https://aflow.org/p/A9BC3_hR26_155_3cdef_c_f-001



Prototype	Al_9ErNi_3
AFLOW prototype label	A9BC3_hR26_155_3cdef_c_f-001
ICSD	105031
Pearson symbol	hR26
Space group number	155
Space group symbol	$R32$
AFLOW prototype command	`aflow --proto=A9BC3_hR26_155_3cdef_c_f-001 --params=`$a, c/a, x_1, x_2, x_3, x_4, y_5, y_6, x_7, y_7, z_7, x_8, y_8, z_8$

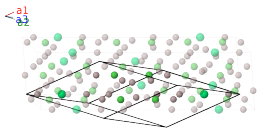
Other compounds with this structure

$DyNi_3Al_9$, $ErNi_3Al_9$, $GdNi_3Al_9$, YNi_3Al_9, $YbNi_3Al_9$, $YbNi_3Ga_9$

- $DyNi_3Al_9$ and YNi_3Al_9 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

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		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

$$\mathbf{B_{24}} = -z_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_8 - z_8)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_8 - 2y_8 + z_8)\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_8 + y_8 + z_8)\;\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Ni I}$$

$$\mathbf{B_{25}} = -y_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(y_8 - z_8)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(2x_8 - y_8 - z_8)\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_8 + y_8 + z_8)\;\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Ni I}$$

$$\mathbf{B_{26}} = -x_8\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 - y_8\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_8 - y_8)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_8 + y_8 - 2z_8)\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(x_8 + y_8 + z_8)\;\hat{\mathbf{z}} \quad \text{(6f)} \quad \text{Ni I}$$

References

[1] R. E. Gladyshevskii, K. Cenzual, H. D. Flack, and E. Parthé, *Structure of RNi_3Al_9 (R = 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.