

La₂Ni₃ Structure:

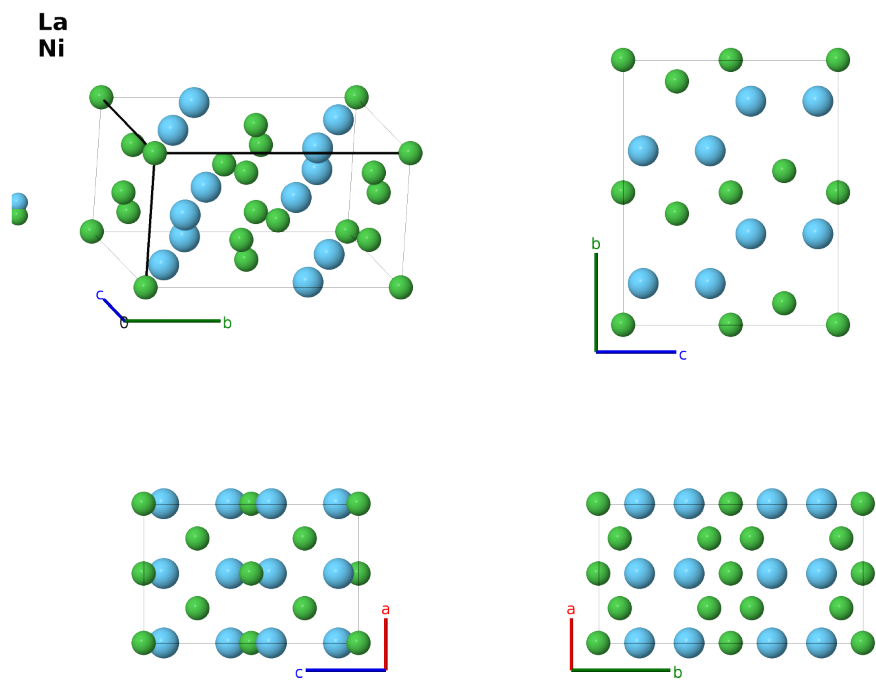
A2B3_oC20_64_f_ae-001

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. Osos, 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/4LJZ>

https://aflow.org/prototype-encyclopedia/A2B3_oC20_64_f_ae-001



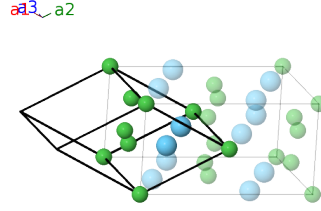
Prototype	La ₂ Ni ₃
AFLOW prototype label	A2B3_oC20_64_f_ae-001
ICSD	450
CCDC	1590969
Pearson symbol	oC20
Space group number	64
Space group symbol	<i>Cmce</i>
AFLOW prototype command	<code>aflow --proto=A2B3_oC20_64_f_ae-001</code> <code>--params=a, b/a, c/a, y₂, y₃, z₃</code>

Other compounds with this structure

K₂Au₃, La₂Co₃, Nd₂Co₃, Rb₂Au₃, GaRh₂Pr₂

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	= 0 =		0	(4a)	Ni I
$\mathbf{B}_2$	= $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$ =		$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4a)	Ni I
$\mathbf{B}_3$	= $-(y_2 - \frac{1}{4}) \mathbf{a}_1 + (y_2 + \frac{1}{4}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$ =		$\frac{1}{4}a \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8e)	Ni II
$\mathbf{B}_4$	= $(y_2 + \frac{1}{4}) \mathbf{a}_1 - (y_2 - \frac{1}{4}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$ =		$\frac{1}{4}a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8e)	Ni II
$\mathbf{B}_5$	= $(y_2 + \frac{3}{4}) \mathbf{a}_1 - (y_2 - \frac{3}{4}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$ =		$\frac{3}{4}a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8e)	Ni II
$\mathbf{B}_6$	= $-(y_2 - \frac{3}{4}) \mathbf{a}_1 + (y_2 + \frac{3}{4}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$ =		$\frac{3}{4}a \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8e)	Ni II
$\mathbf{B}_7$	= $-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$ =		$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8f)	La I
$\mathbf{B}_8$	= $(y_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$ =		$\frac{1}{2}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	La I
$\mathbf{B}_9$	= $-(y_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$ =		$\frac{1}{2}a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	La I
$\mathbf{B}_{10}$	= $y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$ =		$-by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8f)	La I

References

- [1] J. H. N. V. Vucht and K. H. J. Buschow, *The Crystal Structure of La₂Ni₃*, J. Less-Common Met. **46**, 133–138 (1976), doi:10.1016/0022-5088(76)90186-7.

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.