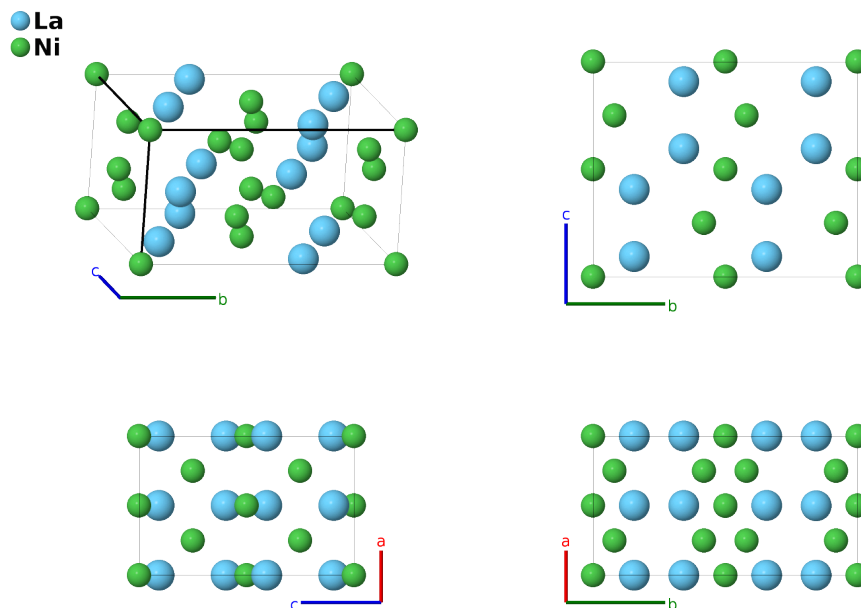


La₂Ni₃ Structure: A2B3_oC20_64_f_ae-001

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<https://afLOW.org/p/4LJZ>

https://afLOW.org/p/A2B3_oC20_64_f_ae-001

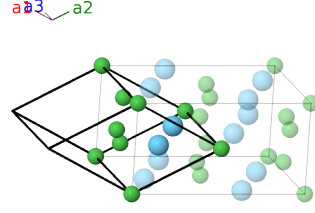


Prototype	La ₂ Ni ₃
AFLOW prototype label	A2B3_oC20_64_f_ae-001
ICSD	450
Pearson symbol	oC20
Space group number	64
Space group symbol	<i>Cmce</i>
AFLOW prototype command	<code>afLOW --proto=A2B3_oC20_64_f_ae-001 --params=a, b/a, c/a, y₂, y₃, z₃</code>

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 La_2Ni_3* , *J. Less-Common Met.* **46**, 133–138 (1976), doi:10.1016/0022-5088(76)90186-7.