

Ga₄Ni Structure:

A4B_cI40_197_cde_c-001

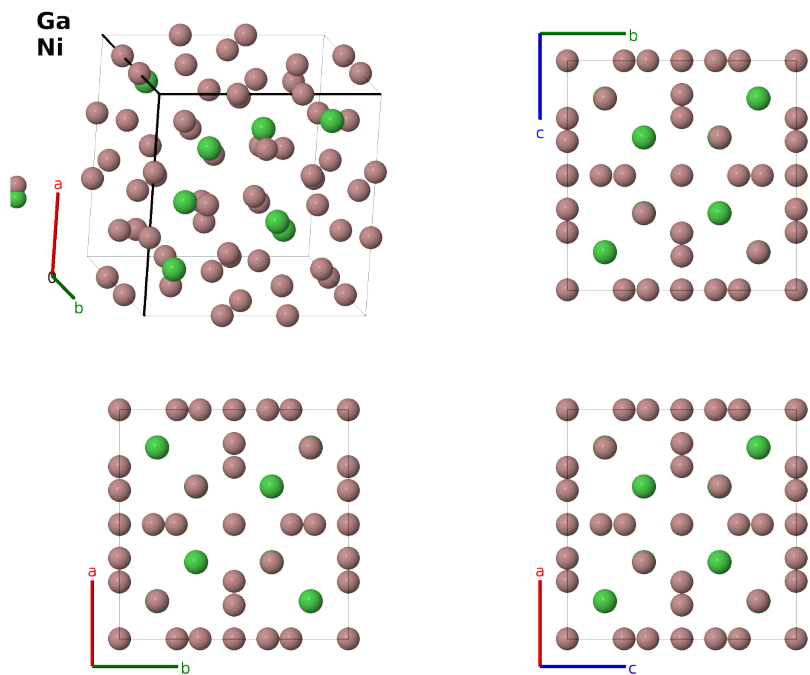
This structure previously used the label(s) **A4B_cI40_197_cde.c**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, 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/PBV9>

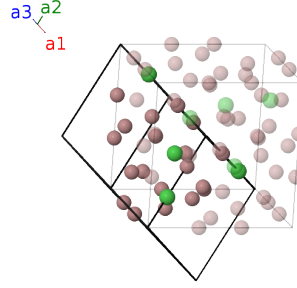
https://aflow.org/prototype-encyclopedia/A4B_cI40_197_cde_c-001



Prototype	Ga ₄ Ni
AFLOW prototype label	A4B_cI40_197_cde_c-001
ICSD	103863
CCDC	1661797
Pearson symbol	cI40
Space group number	197
Space group symbol	I23
AFLOW prototype command	<code>aflow --proto=A4B_cI40_197_cde_c-001</code> <code>--params=a, x₁, x₂, x₃, x₄</code>

Body-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 2x_1 \mathbf{a}_1 + 2x_1 \mathbf{a}_2 + 2x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(8c)	Ga I
$\mathbf{B}_2$	$= -2x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(8c)	Ga I
$\mathbf{B}_3$	$= -2x_1 \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(8c)	Ga I
$\mathbf{B}_4$	$= -2x_1 \mathbf{a}_1$	$=$	$ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(8c)	Ga I
$\mathbf{B}_5$	$= 2x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + 2x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8c)	Ni I
$\mathbf{B}_6$	$= -2x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8c)	Ni I
$\mathbf{B}_7$	$= -2x_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8c)	Ni I
$\mathbf{B}_8$	$= -2x_2 \mathbf{a}_1$	$=$	$ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8c)	Ni I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}}$	(12d)	Ga II
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}}$	(12d)	Ga II
$\mathbf{B}_{11}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{y}}$	(12d)	Ga II
$\mathbf{B}_{12}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{y}}$	(12d)	Ga II
$\mathbf{B}_{13}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{z}}$	(12d)	Ga II
$\mathbf{B}_{14}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{z}}$	(12d)	Ga II
$\mathbf{B}_{15}$	$= \frac{1}{2} \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}$	(12e)	Ga III
$\mathbf{B}_{16}$	$= \frac{1}{2} \mathbf{a}_1 - x_4 \mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}$	(12e)	Ga III
$\mathbf{B}_{17}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(12e)	Ga III
$\mathbf{B}_{18}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(12e)	Ga III
$\mathbf{B}_{19}$	$= x_4 \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + ax_4 \hat{\mathbf{z}}$	(12e)	Ga III
$\mathbf{B}_{20}$	$= -x_4 \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - ax_4 \hat{\mathbf{z}}$	(12e)	Ga III

References

- [1] L. Jingkui and X. Sishen, *The Structure of NiGa₄ Crystal – A New Vacancy Controlled γ -Brass Phase*, Scientia Sinica, Series A **26**, 1305–1313 (1983).

Found in

- [1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017