

Sm₂NiGa₁₂ Structure:

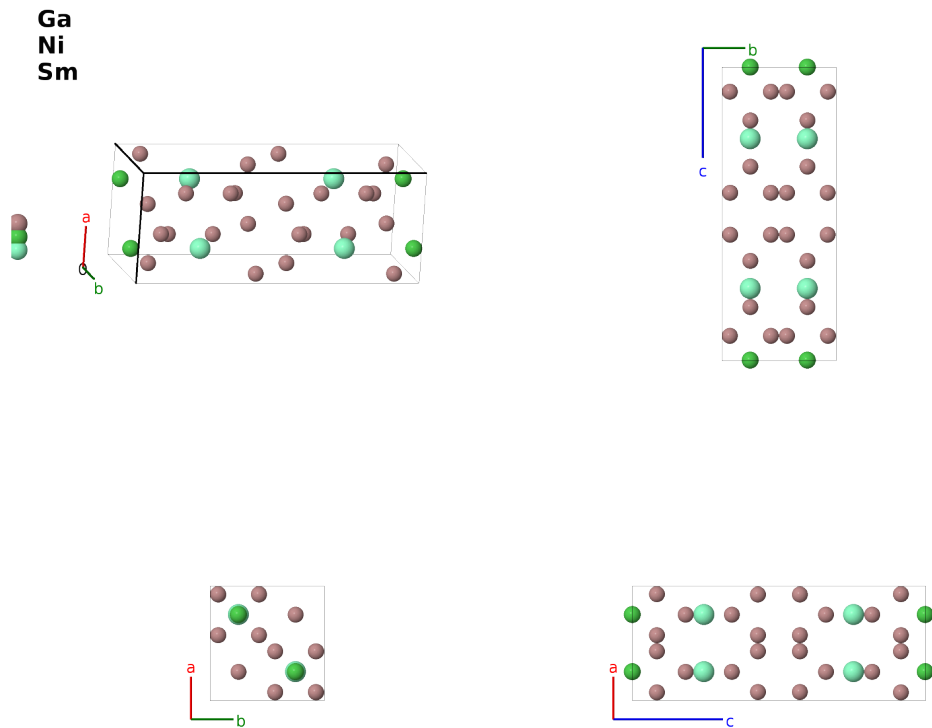
A12BC2_tP30_125_2g2m_c_h-001

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- 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/UYGN>

https://aflow.org/prototype-encyclopedia/A12BC2_tP30_125_2g2m_c_h-001



Prototype	Ga ₁₂ NiSm ₂
AFLOW prototype label	A12BC2_tP30_125_2g2m_c_h-001
Pearson symbol	tP30
Space group number	125
Space group symbol	<i>P4/nbm</i>
AFLOW prototype command	<code>aflow --proto=A12BC2_tP30_125_2g2m_c_h-001</code> <code>--params=a, c/a, z₂, z₃, z₄, x₅, z₅, x₆, z₆</code>

Other compounds with this structure

Ce₂CuGa₁₂, Ce₂IrGa₁₂, Ce₂NiGa₁₂, Ce₂PdGa₁₂, La₂CuGa₁₂, La₂NiGa₁₂, La₂PdGa₁₂, Nd₂CuGa₁₂, Nd₂NiGa₁₂, Nd₂PdGa₁₂, Pr₂CuGa₁₂, Pr₂NiGa₁₂, Pr₂PdGa₁₂, Sm₂CuGa₁₂, Sm₂PdGa₁₂

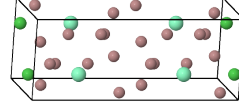
- The ICSD lists Ce₂CuGa₁₂ (ICSD entry 161767, CCDC deposition number 1678129) as the prototype for this structure, but the (Chen, 2000) description of Sm₂NiGa₁₂ predates any description of any other structure with this prototype.

Simple Tetragonal primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(2c)	Ni I
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(2c)	Ni I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4g)	Ga I
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4g)	Ga I
$\mathbf{B}_5$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4g)	Ga I
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4g)	Ga I
$\mathbf{B}_7$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4g)	Ga II
$\mathbf{B}_8$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4g)	Ga II
$\mathbf{B}_9$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4g)	Ga II
$\mathbf{B}_{10}$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4g)	Ga II
$\mathbf{B}_{11}$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4h)	Sm I
$\mathbf{B}_{12}$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4h)	Sm I
$\mathbf{B}_{13}$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4h)	Sm I
$\mathbf{B}_{14}$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4h)	Sm I
$\mathbf{B}_{15}$	$= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8m)	Ga III
$\mathbf{B}_{16}$	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8m)	Ga III
$\mathbf{B}_{17}$	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8m)	Ga III
$\mathbf{B}_{18}$	$= -x_5 \mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8m)	Ga III
$\mathbf{B}_{19}$	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8m)	Ga III
$\mathbf{B}_{20}$	$= x_5 \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8m)	Ga III
$\mathbf{B}_{21}$	$= -x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8m)	Ga III
$\mathbf{B}_{22}$	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8m)	Ga III
$\mathbf{B}_{23}$	$= x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8m)	Ga IV
$\mathbf{B}_{24}$	$= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a\left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8m)	Ga IV
$\mathbf{B}_{25}$	$= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a\left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8m)	Ga IV

$$\begin{aligned}
\mathbf{B}_{26} &= -x_6 \mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right) \mathbf{a}_2 + z_6 \mathbf{a}_3 &= -ax_6 \hat{\mathbf{x}} - a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} &(8m) &\text{Ga IV} \\
\mathbf{B}_{27} &= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(8m) &\text{Ga IV} \\
\mathbf{B}_{28} &= x_6 \mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_2 - z_6 \mathbf{a}_3 &= ax_6 \hat{\mathbf{x}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(8m) &\text{Ga IV} \\
\mathbf{B}_{29} &= -x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -ax_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(8m) &\text{Ga IV} \\
\mathbf{B}_{30} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right) \mathbf{a}_2 - z_6 \mathbf{a}_3 &= a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(8m) &\text{Ga IV}
\end{aligned}$$

References

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- [1] K. R. Thomas, J. Y. Cho, J. N. Millican, R. D. Hembree, M. Moldovan, A. Karki, D. P. Young, and J. Y. Chan, *Crystal growth and physical properties of $\text{Ln}_2\text{MGa}_{12}$ ($\text{Ln}=\text{Pr}$, Nd , and Sm ; $\text{M}=\text{Ni}$, Cu)*, J. Cryst. Growth **312**, 1098–1103 (2010), doi:10.1016/j.jcrysgro.2009.12.039.

First cited in

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