

Y-MgNiSn Structure:

A7B7C2_tP32_101_ade_bde_d-001

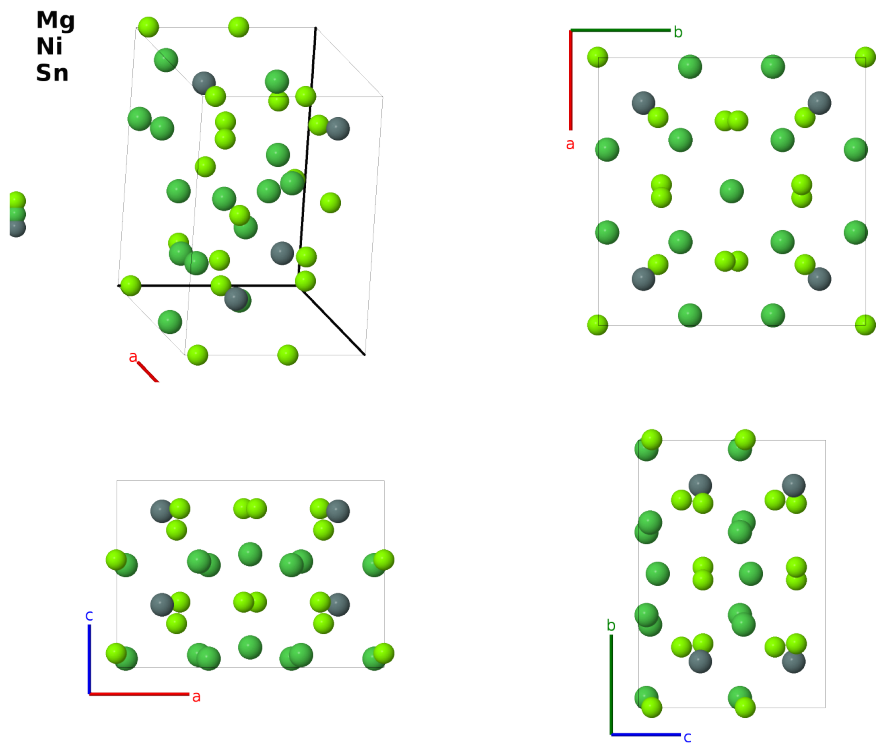
This structure previously used the label(s) **A7B7C2_tP32_101_bde_ade_d**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/LR8K>

https://aflow.org/prototype-encyclopedia/A7B7C2_tP32_101_ade_bde_d-001

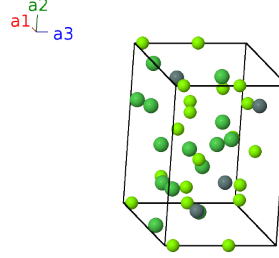


Prototype	MgNiSn
AFLOW prototype label	A7B7C2_tP32_101_ade_bde_d-001
ICSD	99208
CCDC	1658436
Pearson symbol	tP32
Space group number	101
Space group symbol	$P4_2cm$
AFLOW prototype command	<code>aflow --proto=A7B7C2_tP32_101_ade_bde_d-001</code> <code>--params=a, c/a, z₁, z₂, x₃, z₃, x₄, z₄, x₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇</code>

- This is the Y-phase of the Mg-Ni-Sn ternary system. The (2b), (4d) and (8e) Wyckoff positions are partially occupied and are represented by the labels M-I, M-II, and M-III, respectively. Here, M-I is $\text{Mg}_{0.88}\text{Ni}_{0.12}$, which we label “Ni”, M-II is $\text{Sn}_{0.88}\text{Mg}_{0.12}$ labeled “Sn”, and M-III is $\text{Mg}_{0.95}\text{Ni}_{0.05}$, labeled “Ni”, with the supposed element names picked to highlight the different Wyckoff positions.
- We previously referred to this as the γ -phase, but Y-phase is the proper terminology (Boudard, 2004).

Simple Tetragonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	Mg I
$\mathbf{B}_2$	$= \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2a)	Mg I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(2b)	Ni I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2b)	Ni I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4d)	Mg II
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4d)	Mg II
$\mathbf{B}_7$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4d)	Mg II
$\mathbf{B}_8$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4d)	Mg II
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4d)	Ni II
$\mathbf{B}_{10}$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - a x_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4d)	Ni II
$\mathbf{B}_{11}$	$= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4d)	Ni II
$\mathbf{B}_{12}$	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} - a x_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4d)	Ni II
$\mathbf{B}_{13}$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} + a x_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4d)	Sn I
$\mathbf{B}_{14}$	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} - a x_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4d)	Sn I
$\mathbf{B}_{15}$	$= -x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} + a x_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4d)	Sn I
$\mathbf{B}_{16}$	$= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} - a x_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4d)	Sn I
$\mathbf{B}_{17}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a x_6 \hat{\mathbf{x}} + a y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(8e)	Mg III
$\mathbf{B}_{18}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a x_6 \hat{\mathbf{x}} - a y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(8e)	Mg III
$\mathbf{B}_{19}$	$= -y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a y_6 \hat{\mathbf{x}} + a x_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Mg III
$\mathbf{B}_{20}$	$= y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a y_6 \hat{\mathbf{x}} - a x_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Mg III
$\mathbf{B}_{21}$	$= x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_6 \hat{\mathbf{x}} - a y_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Mg III
$\mathbf{B}_{22}$	$= -x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_6 \hat{\mathbf{x}} + a y_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Mg III
$\mathbf{B}_{23}$	$= -y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a y_6 \hat{\mathbf{x}} - a x_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(8e)	Mg III
$\mathbf{B}_{24}$	$= y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a y_6 \hat{\mathbf{x}} + a x_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(8e)	Mg III

$\mathbf{B}_{25}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8e)	Ni III
$\mathbf{B}_{26}$	$=$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8e)	Ni III
$\mathbf{B}_{27}$	$=$	$-y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Ni III
$\mathbf{B}_{28}$	$=$	$y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Ni III
$\mathbf{B}_{29}$	$=$	$x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Ni III
$\mathbf{B}_{30}$	$=$	$-x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Ni III
$\mathbf{B}_{31}$	$=$	$-y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8e)	Ni III
$\mathbf{B}_{32}$	$=$	$y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8e)	Ni III

References

- [1] M. Boudard, P. Bordet, H. Vincent, and F. Audebert, *The structure of the Y-phase in the Mg-Ni-Sn system*, J. Alloys Compd. **372**, 121–128 (2004), doi:10.1016/j.jallcom.2003.09.142.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

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