

Ni₃Sn (*D*₀₁₉) Structure: A3B_hP8_194_h_c-001

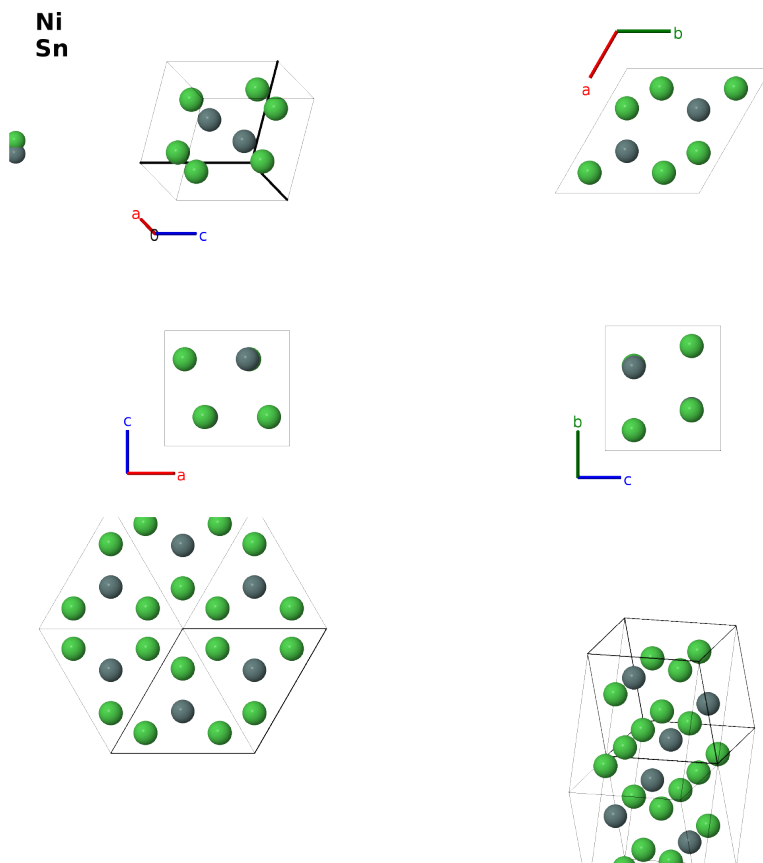
This structure previously used the label(s) **A3B_hP8_194_h_c**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/LJF8>

https://aflow.org/prototype-encyclopedia/A3B_hP8_194_h_c-001



Prototype	Ni ₃ Sn
AFLOW prototype label	A3B_hP8_194_h_c-001
<i>Strukturbericht</i> designation	<i>D</i> ₀₁₉
ICSD	411928
CCDC	1727370
Pearson symbol	hP8
Space group number	194
Space group symbol	<i>P</i> 6 ₃ / <i>mmc</i>

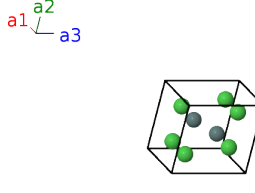
AFLOW prototype command `afLOW --proto=A3B_hP8_194_h_c-001`
 `--params=a, c/a, x2`

Other compounds with this structure

Al₃Gd, Al₃Sm (LT), Al₃Th, Cd₃Mg, Cd₃Sc, Ce₃Al (LT), Co₃Mo, Co₃W, Fe₃Ge (HT), Fe₃Sn, Ga₃Pu (LT), Hg₃Ce, Hg₃Sc, Hg₃Sm, Hg₃Y, Ir₃Mo, Mg₃Cd, Mg₃In, Mn₃Ge, Mn₃Sn, Ni₃In, Ni₃Sn (LT), Pt₃U, Rh₃W, Sc₃In, Ti₃Al, Ti₃Ga, Ti₃Sn (HT), Tl₃Sn, Zn₃Mn

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	Sn I
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	Sn I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Ni I
$\mathbf{B}_4$	$= -2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Ni I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6h)	Ni I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - 2x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Ni I
$\mathbf{B}_7$	$= 2x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Ni I
$\mathbf{B}_8$	$= -x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\sqrt{3}ax_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6h)	Ni I

References

- [1] A. L. Lyubimtsev, A. I. Baranov, A. Fischer, L. Kloo, and B. A. Popovkin, *The structure and bonding of Ni₃Sn*, J. Alloys Compd. **340**, 167–172 (2002), doi:10.1063/1.1662996.

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