Ni_3Sn ($D0_{19}$) Structure: A3B_hP8_194_h_c-001

This structure originally had the label `A3B_hP8_194_h_c`. Calls to that address will be redirected here.

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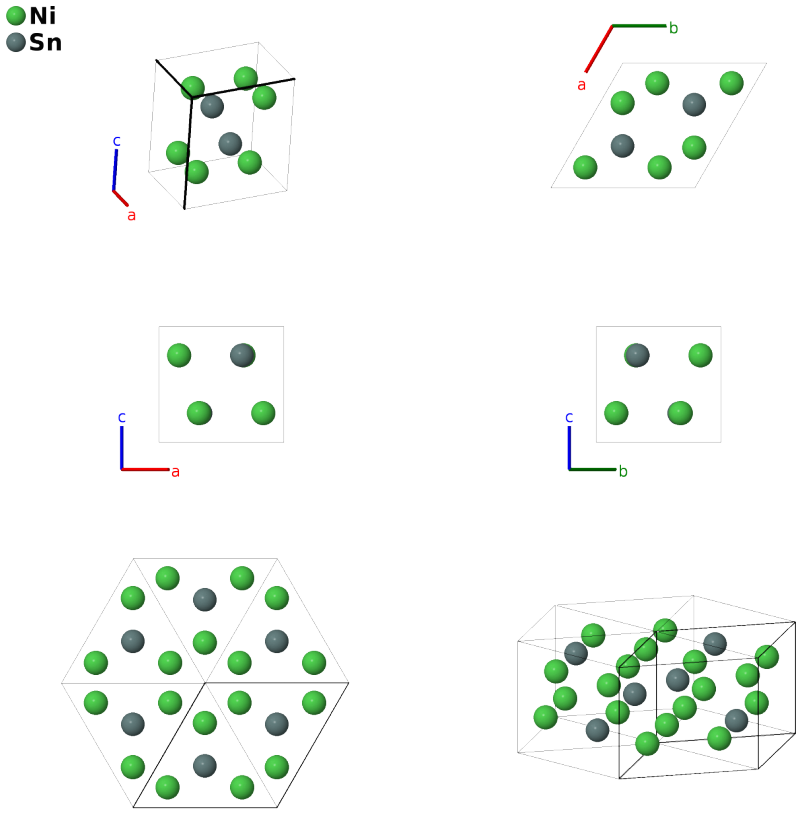
https://aflow.org/p/LJF8

https://aflow.org/p/A3B_hP8_194_h_c-001



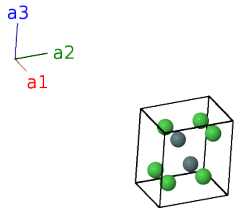
Prototype	Ni_3Sn
AFLOW prototype label	A3B_hP8_194_h_c-001
***Strukturbericht* designation**	$D0_{19}$
ICSD	411928
Pearson symbol	hP8
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=A3B_hP8_194_h_c-001 --params=`$a, c/a, x_2$

Other compounds with this structure

Al_3Gd, Al_3Sm (LT), Al_3Th, Cd_3Mg, Cd_3Sc, Ce_3Al (LT), Co_3Mo, Co_3W, Fe_3Ge (HT), Fe_3Sn, Ga_3Pu (LT), Hg_3Ce, Hg_3Sc, Hg_3Sm, Hg_3Y, Ir_3Mo, Mg_3Cd, Mg_3In, Mn_3Sn, Ni_3In, Ni_3Sn (LT), Pt_3U, Rh_3W, Sc_3In, Ti_3Al, Ti_3Ga, Ti_3Sn (HT), Tl_3Sn, Zn_3Mn

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$



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 Ni_3Sn*, J. Alloys Compd. **340**, 167–172 (2002), doi:10.1063/1.1662996.