δ-Ni_3Sn_4 ($D7_a$) Structure: A3B4_mC14_12_ai_2i-001

This structure originally had the label `A3B4_mC14_12_ai_2i`. Calls to that address will be redirected here.

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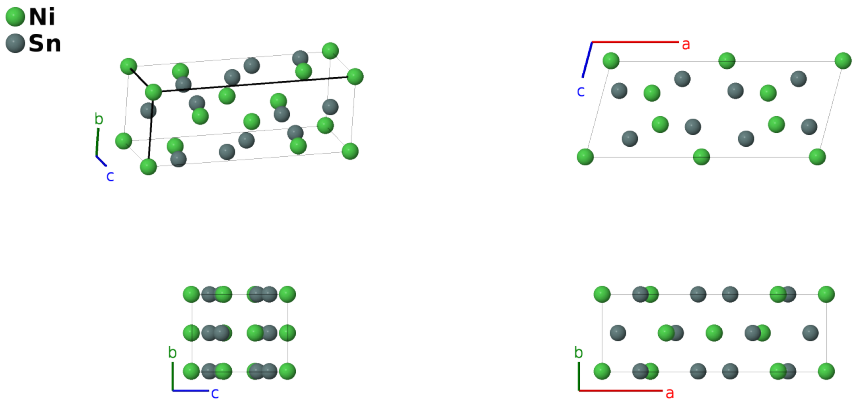
https://aflow.org/p/4WTF

https://aflow.org/p/A3B4_mC14_12_ai_2i-001



Prototype	Ni_3Sn_4
AFLOW prototype label	A3B4_mC14_12_ai_2i-001
***Strukturbericht* designation**	$D7_a$
ICSD	105364
Pearson symbol	mC14
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=A3B4_mC14_12_ai_2i-001 --params=`$a, b/a, c/a, \beta, x_2, z_2, x_3, z_3, x_4, z_4$

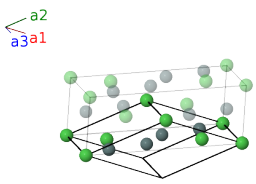
Other compounds with this structure

Cr_3S_4, Cr_3Se_4, Ni_3Sn_4, Fe_3Se_4, Ni_3Se_4, Ti_3Se_4, V_3Se_4, V_3Te_4

- Cr_3Sn_4 and δ-Ni_3Sn_4 ($D7_a$) have the same AFLOW prototype label, A3B4_mC14_12_ai_2i. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ni I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\;\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ni II
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\;\hat{\mathbf{x}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Ni II
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\;\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Sn I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\;\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Sn I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\;\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Sn II
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\;\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Sn II

References

[1] W. Jeitschko and B. Jaberg, *Structure refinement of* Ni_3Sn_4, Acta Crystallogr. Sect. B **38**, 598–600 (1982), doi:10.1107/S056774088200346X.