

δ -Ni₃Sn₄ ($D7_a$) Structure: A3B4_mC14_12_ai_2i-001

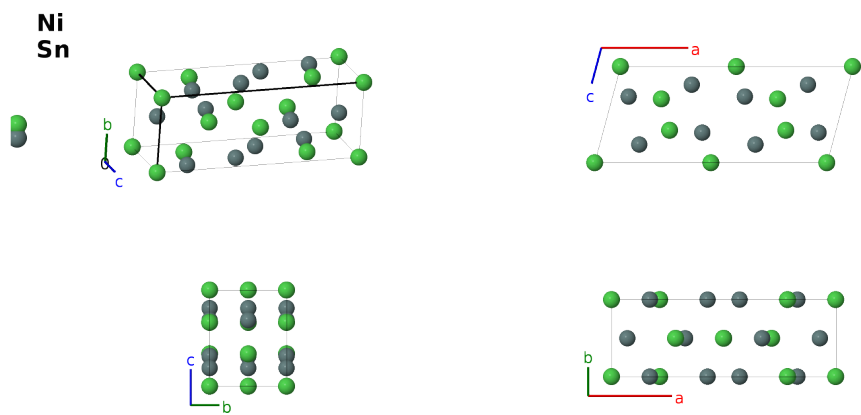
This structure previously used the label(s) **A3B4_mC14_12_ai_2i**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/4WTF>

https://aflow.org/prototype-encyclopedia/A3B4_mC14_12_ai_2i-001



Prototype	Ni ₃ Sn ₄
AFLOW prototype label	A3B4_mC14_12_ai_2i-001
<i>Strukturbericht</i> designation	$D7_a$
ICSD	105364
CCDC	1663253
Pearson symbol	mC14
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<code>aflow --proto=A3B4_mC14_12_ai_2i-001</code> <code>--params=a, b/a, c/a, β, x_2, z_2, x_3, z_3, x_4, z_4</code>

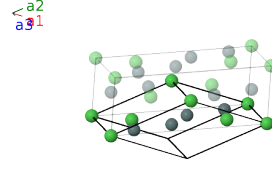
Other compounds with this structure

Cr₃S₄, Cr₃Se₄, Ni₃Sn₄, Fe₃Se₄, Ni₃Se₄, Ti₃Se₄, V₃Se₄, V₃Te₄

- Cr₃S₄ and δ -Ni₃Sn₄ ($D7_a$) 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

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



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. Jäbergh, *Structure refinement of Ni_3Sn_4* , Acta Crystallogr. Sect. B **38**, 598–600 (1982), doi:10.1107/S056774088200346X.

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