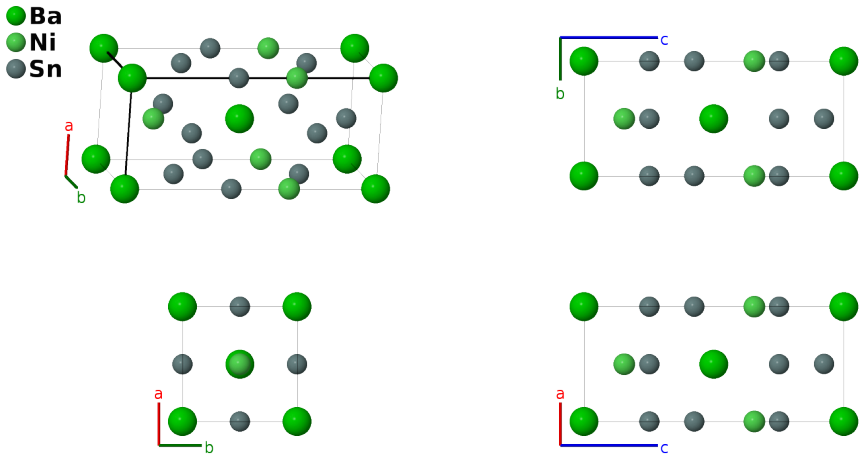
$BaNiSn_3$ Structure: ABC3_tI10_107_a_a_ab-001

This structure originally had the label `ABC3_tI10_107_a_a_ab`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

https://aflow.org/p/N3SR

https://aflow.org/p/ABC3_tI10_107_a_a_ab-001



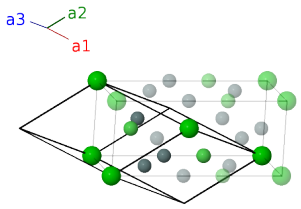
Prototype	$BaNiSn_3$
AFLOW prototype label	ABC3_tI10_107_a_a_ab-001
ICSD	58662
Pearson symbol	tI10
Space group number	107
Space group symbol	$I4mm$
AFLOW prototype command	`aflow --proto=ABC3_tI10_107_a_a_ab-001 --params=`$a, c/a, z_1, z_2, z_3, z_4$

Other compounds with this structure
$BaPdSn_3$, $BaPtSn_3$, $CeCuAl_3$, $EuPdGe_3$, $LaOsSb_3$, $SrIrAl_3$, $SrNiSn_3$, $SrPdAl_3$, $SrPtAl_3$

- This is a ternary form of the $D1_3$ ($BaAl_4$) structure. The atomic positions in both conventional cells are approximately the same, but the distribution of the atoms on those sites and the resulting relaxation leads to a different structure.
- Although (Dörrscheidt, 1978) give the structural information for $BaPtSn_3$ before that of $BaNiSn_3$, (Shatruk, 2019) and others list $BaNiSn_3$ as the prototype for this structure.
- Space group $I4mm$ #107 does not specify the origin of the z-axis. (Dörrscheidt, 1978) places the barium atom at the origin.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Ba I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$cz_2\,\hat{\mathbf{z}}$	(2a)	Ni I
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(2a)	Sn I
$\mathbf{B_4}$	=	$\left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4b)	Sn II
$\mathbf{B_5}$	=	$z_4\,\mathbf{a}_1 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(4b)	Sn II

References

[1] W. Dörrscheidt and H. Schäfer, *Die struktur des $BaPtSn_3$, $BaNiSn_3$ und $SrNiSn_3$ und ihre verwandtschaft zum $ThCr_2Si_2$-strukturtyp*, J. Less-Common Met. **58**, 209–216 (1978), doi:10.1016/0022-5088(78)90202-3.