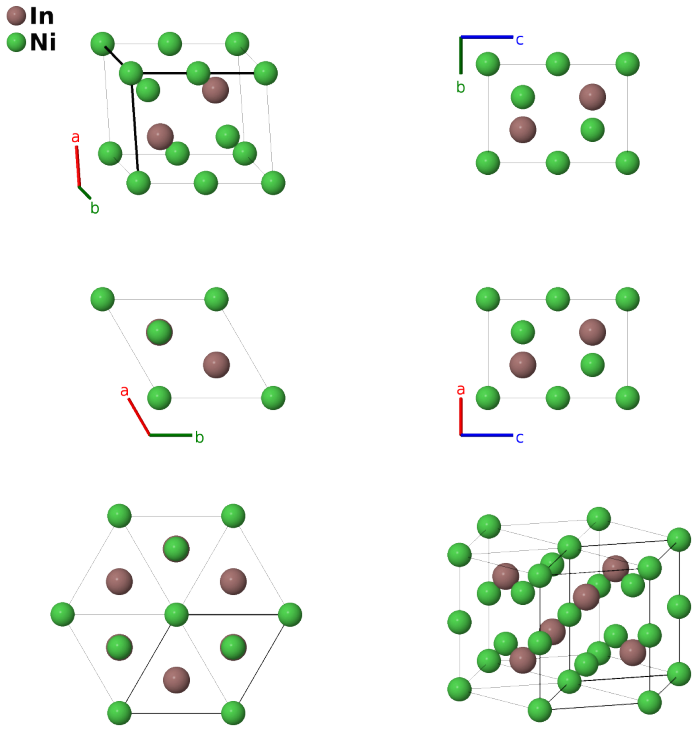
$InNi_2$ ($B8_2$) Structure: AB2_hP6_194_c_ad-001

This structure originally had the label `AB2_hP6_194_c_ad`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/X5ZH

https://aflow.org/p/AB2_hP6_194_c_ad-001



Prototype	$InNi_2$
AFLOW prototype label	AB2_hP6_194_c_ad-001
***Strukturbericht* designation**	$B8_2$
ICSD	59436
Pearson symbol	hP6
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=AB2_hP6_194_c_ad-001 --params=`$a, c/a$

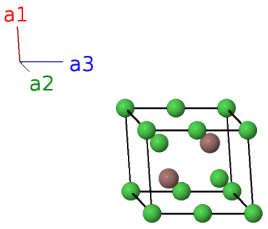
Other compounds with this structure

$AlZr_2$, $BiIn_2$, $GaTi_2$, $SnTi_2$, BeHfSi, BeSiZr, CoFeGe, CoNiGe, CoNiSn, FeGeMn, FeGeNi, GeMnNi

- Replacing the Ni-II atoms with In transforms the crystal into the $C32$ (hexagonal ω) phase.

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
$\mathbf{B_1}$	=	0	=	0	(2a)	Ni I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Ni I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	In I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	In I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2d)	Ni II
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2d)	Ni II

References

[1] M. Ellner, *Über die kristallchemischen parameter der Ni-, Co- und Fe-haltigen phasen vom NiAs-Typ*, J. Less-Common Met. **48**, 21–52 (1976), doi:10.1016/0022-5088(76)90231-9.

Found in

[1] P. Villars, *Ni_2In Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.