Nickeline (NiAs, $B8_1$) Structure: AB_hP4_194_c_a-001

This structure previously used the label(s) `AB_hP4_194_c_a`. Calls to these addresses will be redirected here.

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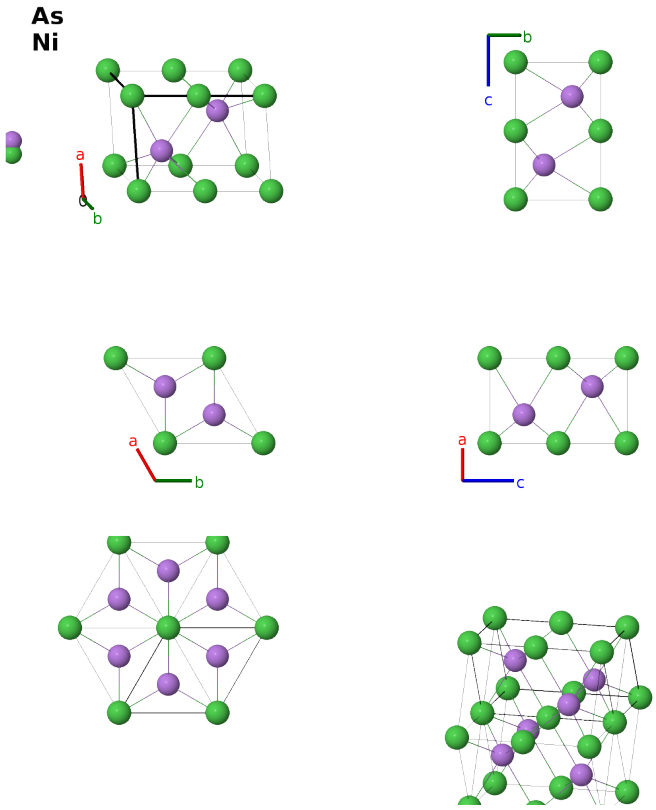
https://aflow.org/prototype-encyclopedia/Y3TN

https://aflow.org/prototype-encyclopedia/AB_hP4_194_c_a-001



Prototype	AsNi
AFLOW prototype label	AB_hP4_194_c_a-001
***Strukturbericht* designation**	$B8_1$
Mineral name	nickeline
ICSD	61104
CCDC	1624650
Pearson symbol	hP4
Space group number	194
Space group symbol	$P6_3/mmc$

AFLOW prototype command `aflow --proto=AB_hP4_194_c_a-001 --params=`$a, c/a$

Other compounds with this structure

AuSn, CoAs, β-CoS, CoSb, CoSe, CoTe, CrH, β-CrSb, CrSe, CuSn, FeS, α-FeSe, α"-FeSe, IrPb, IrS, IrSb, IrSn, IrTe, MgPo, MnAs, MnBi (L.T.), MnSb, MnTe (L.T.), NbS_{1+x}, NiBi, δ-NiS, NiSb, NiSe (H.T.), NiSn, NiTe, PdSb, PdTe, PtB, PtBi, PtPb, PtSb, PtSn, RhSe, RhSn, RhTe, ScSe, ThBi, β-TiAs, TiS, TiSb, TiSc, VP, VS, VSb, VSe, VTe, ZrTe

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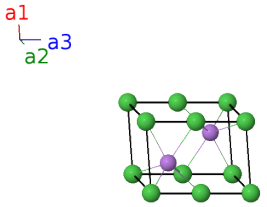
- Note that the stacking is ABACABAC, with the nickel atoms on the A sites and arsenic on B and C. The local environment is fcc-like for nickel atoms and hcp-like for arsenic atoms.
- NiAs $B8_1$ and Fe_2N $L'3_0$ share the same AFLOW prototype label, AB_hP4_194_c_a. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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)	As 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)	As I

References

[1] P. Brand and J. Briest, *Das quasi-binäre System NiAs–$Ni_{1.5}Sn$*, Z. Anorganische und Allgemeine Chemie **337**, 200–204 (1965), doi:10.1002/zaac.19653370314.

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.

First cited in

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