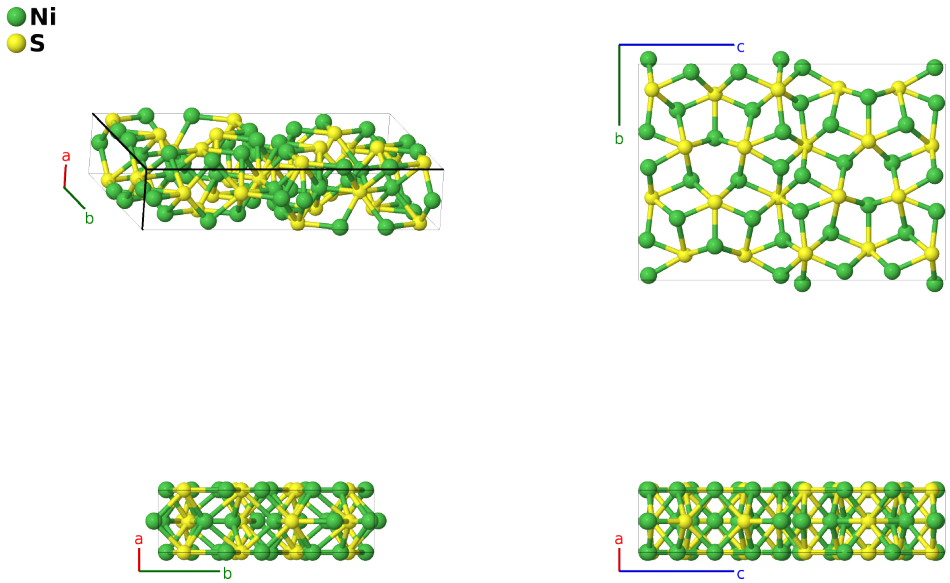
α-Ni_7S_6 Structure: A9B5_oC56_63_c4f_c2f-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/T4VC

https://aflow.org/p/A9B5_oC56_63_c4f_c2f-001



Prototype	Ni_7S_6
AFLOW prototype label	A9B5_oC56_63_c4f_c2f-001
ICSD	2768
Pearson symbol	oC56
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=A9B5_oC56_63_c4f_c2f-001 --params=`$a, b/a, c/a, y_1, y_2, y_3, z_3, y_4, z_4, y_5, z_5, y_6, z_6, y_7, z_7, y_8, z_8$

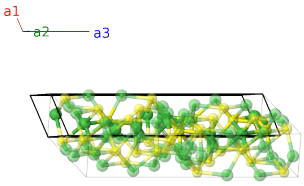
- This structure goes by various names: (Pearson, 1967) calls it Ni_6S_5, while (Villars, 2018) calls it $Ni_{5.6}S_{4.9}$ or γ-Ni_7S_6. This confusion exists because most of the sites are only partially occupied:
  - The Ni I (4c) site has 96.5% occupation.
  - The S I (4c) site is fully occupied.
  - The Ni II (8f) site has 43.6% occupation.
  - The Ni III (8f) site has 91.9% occupation.
  - The Ni IV (8f) site has 51.8% occupation.

  - The Ni V (8f) site has 45.9% occupation.
  - The S I (8f) site has 98.5% occupation.
  - The S II (8f) site has 94.5% occupation.

- Thus the stoichiometry of this system is $Ni_{22.516}S_{19.440}$, $Ni_7S_{6.044}$, or $Ni_{5.6}S_{4.83}$. Allowing for rounding, Ni_7S_6 seems to be the best choice.
- (Villars, 2018) gives this as a high-temperature structure, stable in the range 520-800K, with the exact boundaries depending on the composition.
- (Fleet, 1972) gives the structure in the *Bmmb* setting of space group #63. We used FINDSYM to transform this to the standard *Cmcm* setting.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Ni I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Ni I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8f)	Ni II
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Ni II
$\mathbf{B_7}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Ni II
$\mathbf{B_8}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8f)	Ni II
$\mathbf{B_9}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8f)	Ni III
$\mathbf{B_{10}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Ni III
$\mathbf{B_{11}}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Ni III
$\mathbf{B_{12}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8f)	Ni III
$\mathbf{B_{13}}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8f)	Ni IV
$\mathbf{B_{14}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Ni IV
$\mathbf{B_{15}}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Ni IV
$\mathbf{B_{16}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8f)	Ni IV
$\mathbf{B_{17}}$	=	$-y_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8f)	Ni V
$\mathbf{B_{18}}$	=	$y_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Ni V
$\mathbf{B_{19}}$	=	$-y_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Ni V
$\mathbf{B_{20}}$	=	$y_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8f)	Ni V
$\mathbf{B_{21}}$	=	$-y_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8f)	S II

$\mathbf{B_{22}}$	=	$y_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	S II
$\mathbf{B_{23}}$	=	$-y_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	S II
$\mathbf{B_{24}}$	=	$y_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8f)	S II
$\mathbf{B_{25}}$	=	$-y_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8f)	S III
$\mathbf{B_{26}}$	=	$y_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	S III
$\mathbf{B_{27}}$	=	$-y_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_8\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	S III
$\mathbf{B_{28}}$	=	$y_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(8f)	S III

References

[1] M. E. Fleet, *The Crystal Structure of* α-Ni_7S_6, Acta Crystallogr. Sect. B **28**, 1237–1241 (1972), doi:10.1107/S0567740872004029.

[2] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, Volume 2*, *International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 8 (Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1967).

[3] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Nickel-Sulfur Binary Phase Diagram (1990 Singleton M.). Copyright ©2006-2018 ASM International.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).