

α -Ni₇S₆ Structure:

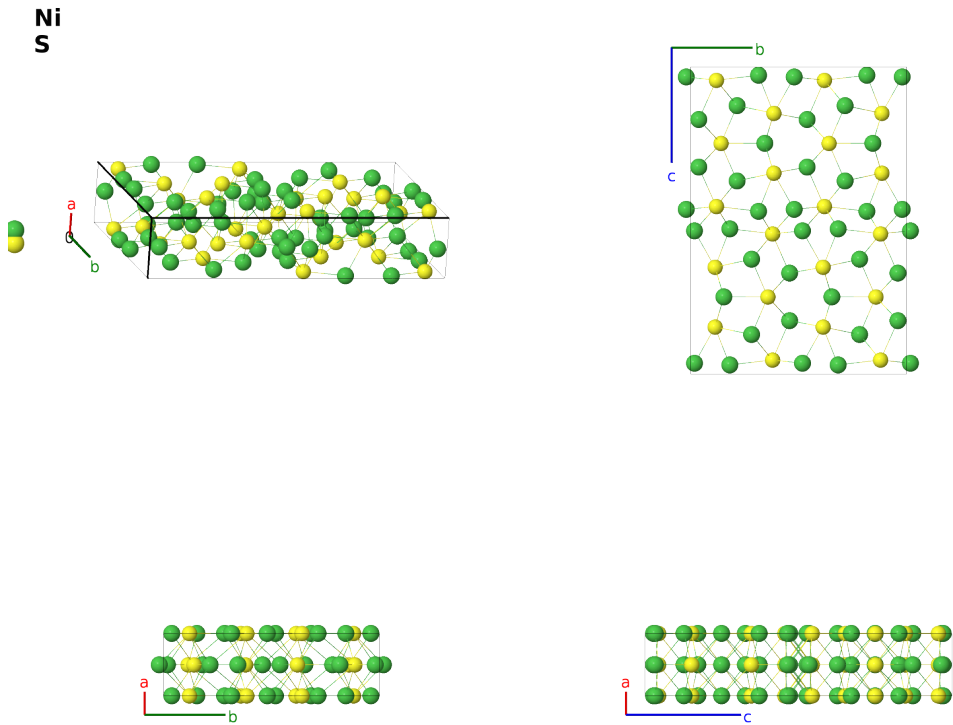
A9B5_oC56_63_c4f_c2f-001

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<https://aflow.org/prototype-encyclopedia/T4VC>

https://aflow.org/prototype-encyclopedia/A9B5_oC56_63_c4f_c2f-001

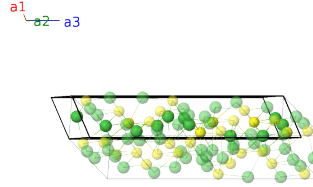


Prototype	Ni ₇ S ₆
AFLOW prototype label	A9B5_oC56_63_c4f_c2f-001
ICSD	2768
CCDC	1592572
Pearson symbol	oC56
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=A9B5_oC56_63_c4f_c2f-001</code> <code>--params=a, b/a, c/a, y₁, y₂, y₃, z₃, y₄, z₄, y₅, z₅, y₆, z₆, y₇, z₇, y₈, z₈</code>

- This structure goes by various names: (Pearson, 1967) calls it Ni_6S_5 , while (Villars, 2018) calls it $\text{Ni}_{5.6}\text{S}_{4.9}$ or $\gamma\text{-Ni}_7\text{S}_6$. 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 $\text{Ni}_{22.516}\text{S}_{19.440}$, $\text{Ni}_7\text{S}_{6.044}$, or $\text{Ni}_{5.6}\text{S}_{4.83}$. 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

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



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
$\mathbf{B}_6$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Ni II
$\mathbf{B}_7$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{10}$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Ni III
$\mathbf{B}_{11}$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(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

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First cited in

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