

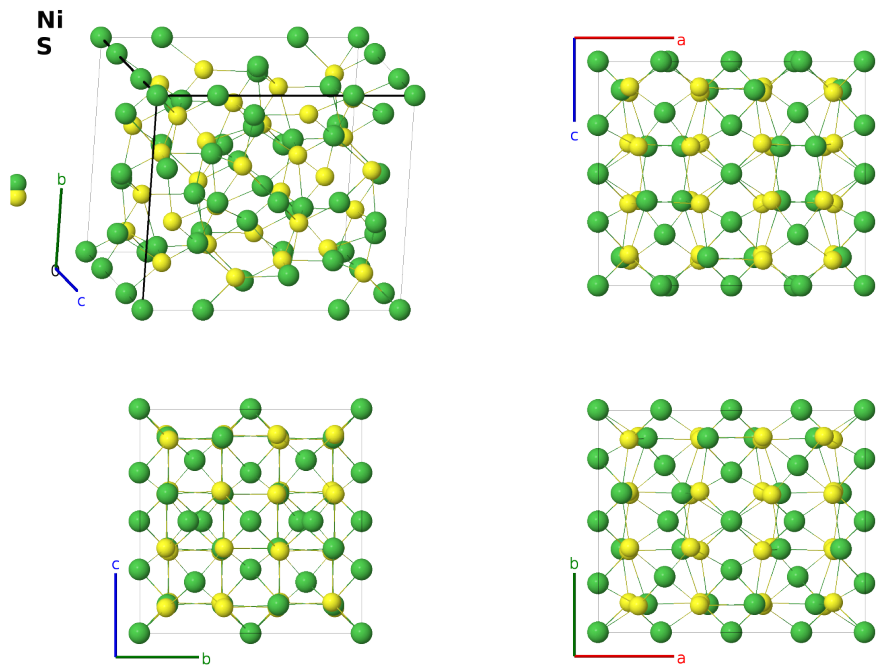
Godlevskite (Ni₉S₈) Structure: A9B8_oC68_21_acehik2l_4l-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/prototype-encyclopedia/L6M4>

https://aflow.org/prototype-encyclopedia/A9B8_oC68_21_acehik2l_4l-001



Prototype	Ni ₉ S ₈
AFLOW prototype label	A9B8_oC68_21_acehik2l_4l-001
Mineral name	godlevskite
ICSD	63080
CCDC	1626227
Pearson symbol	oC68
Space group number	21
Space group symbol	C222
AFLOW prototype command	<pre>aflow --proto=A9B8_oC68_21_acehik2l_4l-001 --params=a, b/a, c/a, x₃, y₄, z₅, z₆, x₇, y₇, z₇, x₈, y₈, z₈, x₉, y₉, z₉, x₁₀, y₁₀, z₁₀, x₁₁, y₁₁, z₁₁, x₁₂, y₁₂, z₁₂</pre>

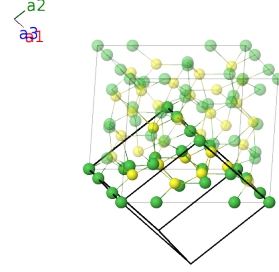
- (Fleet, 1987) says that the actual composition of the sample is $(\text{Ni}_{8.7}\text{Fe}_{0.3})\text{S}_8$ with no information about where the iron atoms are located, although the associated ICSD entry states that our Ni-II (2c) (Fleet's (2b)) site is half nickel and half iron.

Base-centered Orthorhombic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(2a)	Ni I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2c)	Ni II
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}}$	(4e)	Ni III
$\mathbf{B}_4$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}}$	(4e)	Ni III
$\mathbf{B}_5$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h)	Ni IV
$\mathbf{B}_6$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h)	Ni IV
$\mathbf{B}_7$	$= z_5 \mathbf{a}_3$	$=$	$cz_5 \hat{\mathbf{z}}$	(4i)	Ni V
$\mathbf{B}_8$	$= -z_5 \mathbf{a}_3$	$=$	$-cz_5 \hat{\mathbf{z}}$	(4i)	Ni V
$\mathbf{B}_9$	$= \frac{1}{2} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4k)	Ni VI
$\mathbf{B}_{10}$	$= \frac{1}{2} \mathbf{a}_1 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4k)	Ni VI
$\mathbf{B}_{11}$	$= (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8l)	Ni VII
$\mathbf{B}_{12}$	$= -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8l)	Ni VII
$\mathbf{B}_{13}$	$= -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8l)	Ni VII
$\mathbf{B}_{14}$	$= (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8l)	Ni VII
$\mathbf{B}_{15}$	$= (x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8l)	Ni VIII
$\mathbf{B}_{16}$	$= -(x_8 - y_8) \mathbf{a}_1 - (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8l)	Ni VIII
$\mathbf{B}_{17}$	$= -(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8l)	Ni VIII
$\mathbf{B}_{18}$	$= (x_8 + y_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8l)	Ni VIII
$\mathbf{B}_{19}$	$= (x_9 - y_9) \mathbf{a}_1 + (x_9 + y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8l)	S I

$$\begin{aligned}
\mathbf{B}_{20} &= \begin{matrix} -(x_9 - y_9) \mathbf{a}_1 - (x_9 + y_9) \mathbf{a}_2 + \\ z_9 \mathbf{a}_3 \end{matrix} = -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (81) & \text{S I} \\
\mathbf{B}_{21} &= \begin{matrix} -(x_9 + y_9) \mathbf{a}_1 - (x_9 - y_9) \mathbf{a}_2 - \\ z_9 \mathbf{a}_3 \end{matrix} = -ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (81) & \text{S I} \\
\mathbf{B}_{22} &= \begin{matrix} (x_9 + y_9) \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 - \\ z_9 \mathbf{a}_3 \end{matrix} = ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (81) & \text{S I} \\
\mathbf{B}_{23} &= \begin{matrix} (x_{10} - y_{10}) \mathbf{a}_1 + \\ (x_{10} + y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 \end{matrix} = ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (81) & \text{S II} \\
\mathbf{B}_{24} &= \begin{matrix} -(x_{10} - y_{10}) \mathbf{a}_1 - \\ (x_{10} + y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 \end{matrix} = -ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (81) & \text{S II} \\
\mathbf{B}_{25} &= \begin{matrix} -(x_{10} + y_{10}) \mathbf{a}_1 - \\ (x_{10} - y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3 \end{matrix} = -ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (81) & \text{S II} \\
\mathbf{B}_{26} &= \begin{matrix} (x_{10} + y_{10}) \mathbf{a}_1 + \\ (x_{10} - y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3 \end{matrix} = ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (81) & \text{S II} \\
\mathbf{B}_{27} &= \begin{matrix} (x_{11} - y_{11}) \mathbf{a}_1 + \\ (x_{11} + y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3 \end{matrix} = ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (81) & \text{S III} \\
\mathbf{B}_{28} &= \begin{matrix} -(x_{11} - y_{11}) \mathbf{a}_1 - \\ (x_{11} + y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3 \end{matrix} = -ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (81) & \text{S III} \\
\mathbf{B}_{29} &= \begin{matrix} -(x_{11} + y_{11}) \mathbf{a}_1 - \\ (x_{11} - y_{11}) \mathbf{a}_2 - z_{11} \mathbf{a}_3 \end{matrix} = -ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (81) & \text{S III} \\
\mathbf{B}_{30} &= \begin{matrix} (x_{11} + y_{11}) \mathbf{a}_1 + \\ (x_{11} - y_{11}) \mathbf{a}_2 - z_{11} \mathbf{a}_3 \end{matrix} = ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (81) & \text{S III} \\
\mathbf{B}_{31} &= \begin{matrix} (x_{12} - y_{12}) \mathbf{a}_1 + \\ (x_{12} + y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3 \end{matrix} = ax_{12} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (81) & \text{S IV} \\
\mathbf{B}_{32} &= \begin{matrix} -(x_{12} - y_{12}) \mathbf{a}_1 - \\ (x_{12} + y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3 \end{matrix} = -ax_{12} \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (81) & \text{S IV} \\
\mathbf{B}_{33} &= \begin{matrix} -(x_{12} + y_{12}) \mathbf{a}_1 - \\ (x_{12} - y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3 \end{matrix} = -ax_{12} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}} & (81) & \text{S IV} \\
\mathbf{B}_{34} &= \begin{matrix} (x_{12} + y_{12}) \mathbf{a}_1 + \\ (x_{12} - y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3 \end{matrix} = ax_{12} \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}} & (81) & \text{S IV}
\end{aligned}$$

References

- [1] M. E. Fleet, *Structure of Godlevskite, Ni_9S_8* , Acta Crystallogr. Sect. C **43**, 2255–2257 (1987), doi:10.1107/S0108270187088176.

Found in

- [1] 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.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.