Godlevskite (Ni_9S_8) Structure: A9B8_oC68_21_acehik2l_4l-001

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https://aflow.org/p/L6M4

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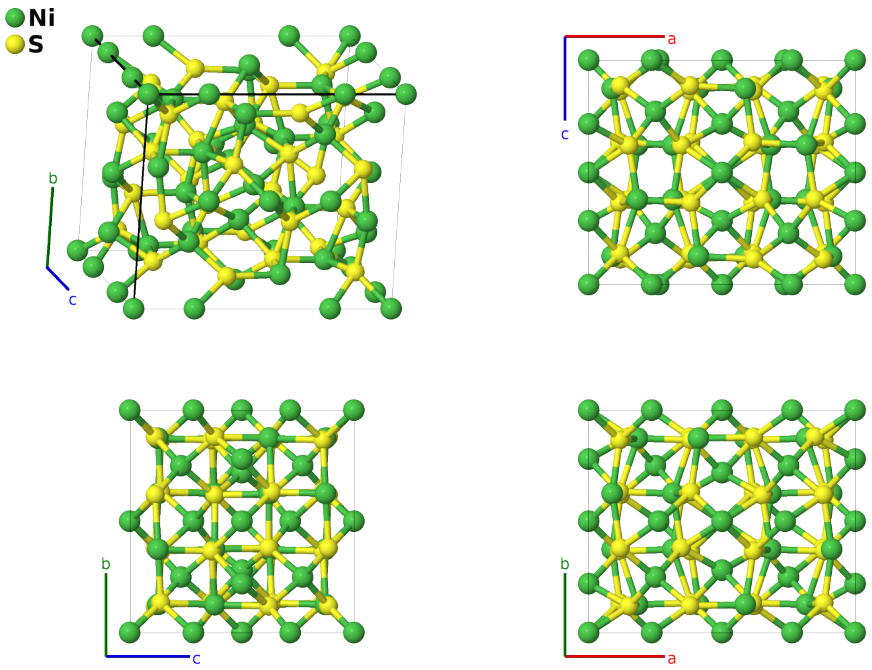
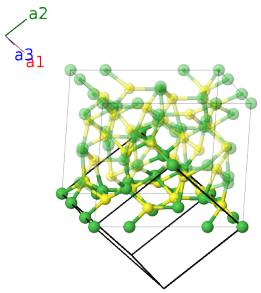


Prototype	Ni_9S_8
AFLOW prototype label	A9B8_oC68_21_acehik2l_4l-001
Mineral name	godlevskite
ICSD	63080
Pearson symbol	oC68
Space group number	21
Space group symbol	$C222$
AFLOW prototype command	`aflow --proto=A9B8_oC68_21_acehik2l_4l-001 --params=`$a, b/a, c/a, x_3, y_4, z_5, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}$

- (Fleet, 1987) says that the actual composition of the sample is $(Ni_{8.7}Fe_{0.3})S_8$ 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

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	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
$\mathbf{B_{20}}$	=	$-(x_9 - y_9)\,\mathbf{a}_1 - (x_9 + y_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(8l)	S I
$\mathbf{B_{21}}$	=	$-(x_9 + y_9)\,\mathbf{a}_1 - (x_9 - y_9)\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(8l)	S I

$$\mathbf{B_{22}} = (x_9 + y_9)\,\mathbf{a}_1 + (x_9 - y_9)\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 = a x_9\,\hat{\mathbf{x}} - b y_9\,\hat{\mathbf{y}} - c z_9\,\hat{\mathbf{z}} \quad (8l) \quad \text{S I}$$

$$\mathbf{B_{23}} = (x_{10} - y_{10})\,\mathbf{a}_1 + (x_{10} + y_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = a x_{10}\,\hat{\mathbf{x}} + b y_{10}\,\hat{\mathbf{y}} + c z_{10}\,\hat{\mathbf{z}} \quad (8l) \quad \text{S II}$$

$$\mathbf{B_{24}} = -(x_{10} - y_{10})\,\mathbf{a}_1 - (x_{10} + y_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = -a x_{10}\,\hat{\mathbf{x}} - b y_{10}\,\hat{\mathbf{y}} + c z_{10}\,\hat{\mathbf{z}} \quad (8l) \quad \text{S II}$$

$$\mathbf{B_{25}} = -(x_{10} + y_{10})\,\mathbf{a}_1 - (x_{10} - y_{10})\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 = -a x_{10}\,\hat{\mathbf{x}} + b y_{10}\,\hat{\mathbf{y}} - c z_{10}\,\hat{\mathbf{z}} \quad (8l) \quad \text{S II}$$

$$\mathbf{B_{26}} = (x_{10} + y_{10})\,\mathbf{a}_1 + (x_{10} - y_{10})\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 = a x_{10}\,\hat{\mathbf{x}} - b y_{10}\,\hat{\mathbf{y}} - c z_{10}\,\hat{\mathbf{z}} \quad (8l) \quad \text{S II}$$

$$\mathbf{B_{27}} = (x_{11} - y_{11})\,\mathbf{a}_1 + (x_{11} + y_{11})\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = a x_{11}\,\hat{\mathbf{x}} + b y_{11}\,\hat{\mathbf{y}} + c z_{11}\,\hat{\mathbf{z}} \quad (8l) \quad \text{S III}$$

$$\mathbf{B_{28}} = -(x_{11} - y_{11})\,\mathbf{a}_1 - (x_{11} + y_{11})\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = -a x_{11}\,\hat{\mathbf{x}} - b y_{11}\,\hat{\mathbf{y}} + c z_{11}\,\hat{\mathbf{z}} \quad (8l) \quad \text{S III}$$

$$\mathbf{B_{29}} = -(x_{11} + y_{11})\,\mathbf{a}_1 - (x_{11} - y_{11})\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 = -a x_{11}\,\hat{\mathbf{x}} + b y_{11}\,\hat{\mathbf{y}} - c z_{11}\,\hat{\mathbf{z}} \quad (8l) \quad \text{S III}$$

$$\mathbf{B_{30}} = (x_{11} + y_{11})\,\mathbf{a}_1 + (x_{11} - y_{11})\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 = a x_{11}\,\hat{\mathbf{x}} - b y_{11}\,\hat{\mathbf{y}} - c z_{11}\,\hat{\mathbf{z}} \quad (8l) \quad \text{S III}$$

$$\mathbf{B_{31}} = (x_{12} - y_{12})\,\mathbf{a}_1 + (x_{12} + y_{12})\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = a x_{12}\,\hat{\mathbf{x}} + b y_{12}\,\hat{\mathbf{y}} + c z_{12}\,\hat{\mathbf{z}} \quad (8l) \quad \text{S IV}$$

$$\mathbf{B_{32}} = -(x_{12} - y_{12})\,\mathbf{a}_1 - (x_{12} + y_{12})\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = -a x_{12}\,\hat{\mathbf{x}} - b y_{12}\,\hat{\mathbf{y}} + c z_{12}\,\hat{\mathbf{z}} \quad (8l) \quad \text{S IV}$$

$$\mathbf{B_{33}} = -(x_{12} + y_{12})\,\mathbf{a}_1 - (x_{12} - y_{12})\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3 = -a x_{12}\,\hat{\mathbf{x}} + b y_{12}\,\hat{\mathbf{y}} - c z_{12}\,\hat{\mathbf{z}} \quad (8l) \quad \text{S IV}$$

$$\mathbf{B_{34}} = (x_{12} + y_{12})\,\mathbf{a}_1 + (x_{12} - y_{12})\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3 = a x_{12}\,\hat{\mathbf{x}} - b y_{12}\,\hat{\mathbf{y}} - c z_{12}\,\hat{\mathbf{z}} \quad (8l) \quad \text{S IV}$$

References

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

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[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.