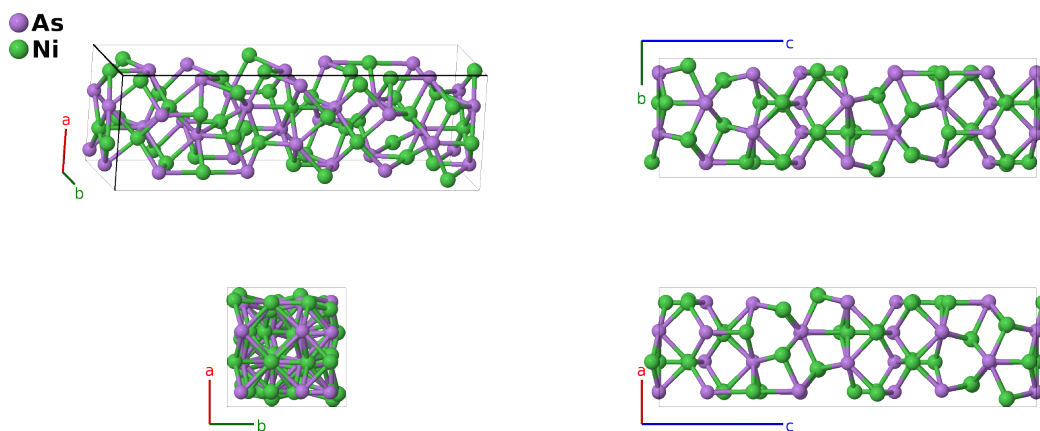


Maucherite (Ni₁₁As₈) Structure: A8B11_tP76_92_2a3b_a5b-001

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<https://afLOW.org/p/CBJ0>

https://afLOW.org/p/A8B11_tP76_92_2a3b_a5b-001



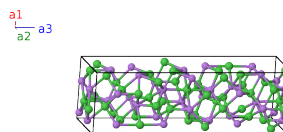
Prototype	As ₈ Ni ₁₁
AFLOW prototype label	A8B11_tP76_92_2a3b_a5b-001
Mineral name	maucherite
ICSD	34853
Pearson symbol	tP76
Space group number	92
Space group symbol	<i>P</i> 4 ₁ 2 ₁ 2
AFLOW prototype command	<code>afLOW --proto=A8B11_tP76_92_2a3b_a5b-001 --params=a, c/a, x₁, x₂, x₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈, x₉, y₉, z₉, x₁₀, y₁₀, z₁₀, x₁₁, y₁₁, z₁₁</code>

Simple Tetragonal primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1 =$	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	$=$	$a x_1 \hat{\mathbf{x}} + a x_1 \hat{\mathbf{y}}$	(4a)	As I

$$\begin{aligned}
\mathbf{B}_{63} &= -\left(y_{10} - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{10} + \frac{1}{4}\right) \mathbf{a}_3 = -a\left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Ni V} \\
\mathbf{B}_{64} &= \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{10} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{10} + \frac{3}{4}\right) \mathbf{a}_3 = a\left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{10} + \frac{3}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Ni V} \\
\mathbf{B}_{65} &= -\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{10} - \frac{1}{4}\right) \mathbf{a}_3 = -a\left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Ni V} \\
\mathbf{B}_{66} &= \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{10} - \frac{3}{4}\right) \mathbf{a}_3 = a\left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{10} - \frac{3}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Ni V} \\
\mathbf{B}_{67} &= y_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 = ay_{10} \hat{\mathbf{x}} + ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (8b) & \text{Ni V} \\
\mathbf{B}_{68} &= -y_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3 = -ay_{10} \hat{\mathbf{x}} - ax_{10} \hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8b) & \text{Ni V} \\
\mathbf{B}_{69} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = ax_{11} \hat{\mathbf{x}} + ay_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8b) & \text{Ni VI} \\
\mathbf{B}_{70} &= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3 = -ax_{11} \hat{\mathbf{x}} - ay_{11} \hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8b) & \text{Ni VI} \\
\mathbf{B}_{71} &= -\left(y_{11} - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_{11} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{11} + \frac{1}{4}\right) \mathbf{a}_3 = -a\left(y_{11} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_{11} + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Ni VI} \\
\mathbf{B}_{72} &= \left(y_{11} + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{11} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{11} + \frac{3}{4}\right) \mathbf{a}_3 = a\left(y_{11} + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{11} + \frac{3}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Ni VI} \\
\mathbf{B}_{73} &= -\left(x_{11} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{11} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{11} - \frac{1}{4}\right) \mathbf{a}_3 = -a\left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_{11} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{11} - \frac{1}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Ni VI} \\
\mathbf{B}_{74} &= \left(x_{11} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{11} - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{11} - \frac{3}{4}\right) \mathbf{a}_3 = a\left(x_{11} + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_{11} - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{11} - \frac{3}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Ni VI} \\
\mathbf{B}_{75} &= y_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 = ay_{11} \hat{\mathbf{x}} + ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (8b) & \text{Ni VI} \\
\mathbf{B}_{76} &= -y_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 - \left(z_{11} - \frac{1}{2}\right) \mathbf{a}_3 = -ay_{11} \hat{\mathbf{x}} - ax_{11} \hat{\mathbf{y}} - c\left(z_{11} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8b) & \text{Ni VI}
\end{aligned}$$

References

- [1] M. E. Fleet, *The Crystal Structure of Maucherite* ($\text{Ni}_{11}\text{As}_8$), *Am. Mineral.* **58**, 203–210 (1973).

Found in

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