

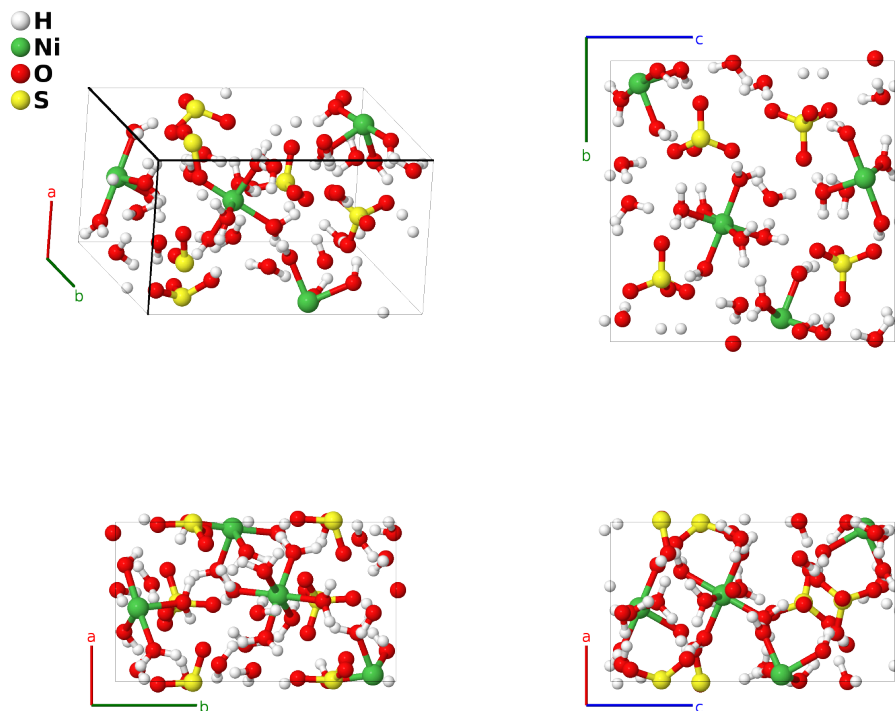
Morenosite ($\text{NiSO}_4 \cdot 7\text{H}_2\text{O}$, $H4_{12}$) Structure: A14BC11D_oP108_19_14a_a_11a_a-001

This structure originally had the label A14BC11D_oP108_19_14a_a_11a_a. Calls to that address will be redirected here.

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<https://aflow.org/p/S9KY>

https://aflow.org/p/A14BC11D_oP108_19_14a_a_11a_a-001



Prototype	$\text{H}_{14}\text{NiO}_{11}\text{S}$
AFLOW prototype label	A14BC11D_oP108_19_14a_a_11a_a-001
<i>Strukturbericht</i> designation	$H4_{12}$
Mineral name	morenosite
ICSD	84569
Pearson symbol	oP108
Space group number	19
Space group symbol	$P2_12_12_1$
AFLOW prototype command	<pre>aflow --proto=A14BC11D_oP108_19_14a_a_11a_a-001 --params=a, b/a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12, x13, y13, z13, x14, y14, z14, x15, y15, z15, x16, y16, z16, x17, y17, z17, x18, y18, z18, x19, y19, z19, x20, y20, z20, x21, y21, z21, x22, y22, z22, x23, y23, z23, x24, y24, z24, x25, y25, z25, x26, y26, z26, x27, y27, z27</pre>

Other compounds with this structure

MgSO₄·7H₂O (Epsomite), ZnSO₄·7H₂O (Gosalrite)

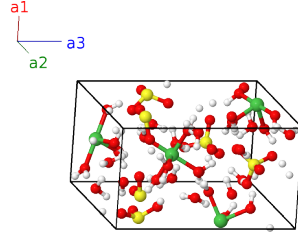
- We use the structure from the 25K neutron data taken by (Ptasiewicz-Bak, 1997).
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Simple Orthorhombic primitive vectors

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

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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4a)	H I
\mathbf{B}_2	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	H I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	H I
\mathbf{B}_4	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4a)	H I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4a)	H II
\mathbf{B}_6	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	H II
\mathbf{B}_7	$= -x_2 \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	H II
\mathbf{B}_8	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4a)	H II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4a)	H III
\mathbf{B}_{10}	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	H III
\mathbf{B}_{11}	$= -x_3 \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	H III
\mathbf{B}_{12}	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4a)	H III
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4a)	H IV
\mathbf{B}_{14}	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	H IV
\mathbf{B}_{15}	$= -x_4 \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	H IV
\mathbf{B}_{16}	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4a)	H IV
\mathbf{B}_{17}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4a)	H V

$$\begin{aligned}
\mathbf{B}_{98} &= -\left(x_{25} - \frac{1}{2}\right) \mathbf{a}_1 - y_{25} \mathbf{a}_2 + \left(z_{25} + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_{25} - \frac{1}{2}\right) \hat{\mathbf{x}} - by_{25} \hat{\mathbf{y}} + c\left(z_{25} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4a) & \text{O X} \\
\mathbf{B}_{99} &= -x_{25} \mathbf{a}_1 + \left(y_{25} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{25} - \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{25} \hat{\mathbf{x}} + b\left(y_{25} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{25} - \frac{1}{2}\right) \hat{\mathbf{z}} &(4a) & \text{O X} \\
\mathbf{B}_{100} &= \left(x_{25} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{25} - \frac{1}{2}\right) \mathbf{a}_2 - z_{25} \mathbf{a}_3 &= a\left(x_{25} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{25} - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{25} \hat{\mathbf{z}} &(4a) & \text{O X} \\
\mathbf{B}_{101} &= x_{26} \mathbf{a}_1 + y_{26} \mathbf{a}_2 + z_{26} \mathbf{a}_3 &= ax_{26} \hat{\mathbf{x}} + by_{26} \hat{\mathbf{y}} + cz_{26} \hat{\mathbf{z}} &(4a) & \text{O XI} \\
\mathbf{B}_{102} &= -\left(x_{26} - \frac{1}{2}\right) \mathbf{a}_1 - y_{26} \mathbf{a}_2 + \left(z_{26} + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_{26} - \frac{1}{2}\right) \hat{\mathbf{x}} - by_{26} \hat{\mathbf{y}} + c\left(z_{26} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4a) & \text{O XI} \\
\mathbf{B}_{103} &= -x_{26} \mathbf{a}_1 + \left(y_{26} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{26} - \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{26} \hat{\mathbf{x}} + b\left(y_{26} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{26} - \frac{1}{2}\right) \hat{\mathbf{z}} &(4a) & \text{O XI} \\
\mathbf{B}_{104} &= \left(x_{26} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{26} - \frac{1}{2}\right) \mathbf{a}_2 - z_{26} \mathbf{a}_3 &= a\left(x_{26} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{26} - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{26} \hat{\mathbf{z}} &(4a) & \text{O XI} \\
\mathbf{B}_{105} &= x_{27} \mathbf{a}_1 + y_{27} \mathbf{a}_2 + z_{27} \mathbf{a}_3 &= ax_{27} \hat{\mathbf{x}} + by_{27} \hat{\mathbf{y}} + cz_{27} \hat{\mathbf{z}} &(4a) & \text{S I} \\
\mathbf{B}_{106} &= -\left(x_{27} - \frac{1}{2}\right) \mathbf{a}_1 - y_{27} \mathbf{a}_2 + \left(z_{27} + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_{27} - \frac{1}{2}\right) \hat{\mathbf{x}} - by_{27} \hat{\mathbf{y}} + c\left(z_{27} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4a) & \text{S I} \\
\mathbf{B}_{107} &= -x_{27} \mathbf{a}_1 + \left(y_{27} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{27} - \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{27} \hat{\mathbf{x}} + b\left(y_{27} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{27} - \frac{1}{2}\right) \hat{\mathbf{z}} &(4a) & \text{S I} \\
\mathbf{B}_{108} &= \left(x_{27} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{27} - \frac{1}{2}\right) \mathbf{a}_2 - z_{27} \mathbf{a}_3 &= a\left(x_{27} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{27} - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{27} \hat{\mathbf{z}} &(4a) & \text{S I}
\end{aligned}$$

References

- [1] H. Ptasiwicz-Bak, I. Olovsson, and G. J. McIntyre, *Charge Density in Orthorhombic NiSO₄·7H₂O at Room Temperature and 25 K*, Acta Crystallogr. Sect. B **53**, 325–336 (1997), doi:10.1107/S0108768196014061.