

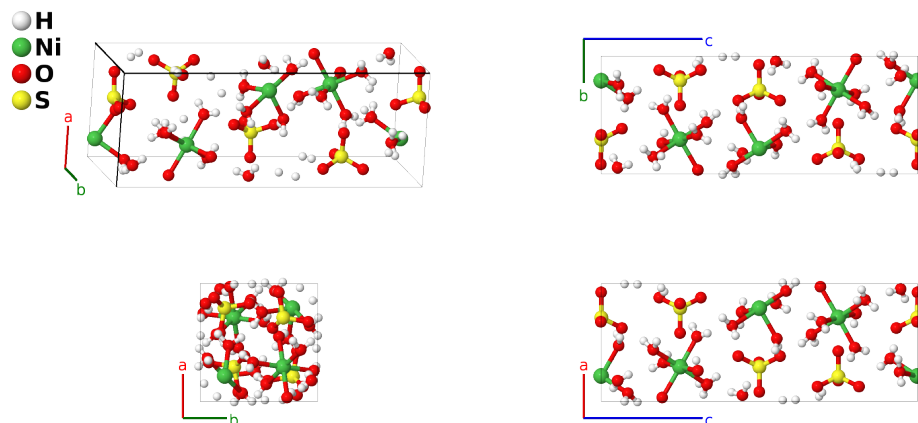
Retgersite (α -NiSO₄·6H₂O, $H4_5$) Structure: A12BC10D_tP96_92_6b_a_5b_a-001

This structure originally had the label A12BC10D_tP96_92_6b_a_5b_a. Calls to that address will be redirected here.

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

https://aflow.org/p/A12BC10D_tP96_92_6b_a_5b_a-001

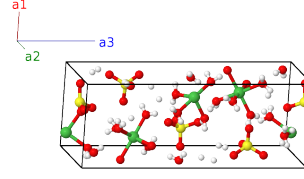


Prototype	H ₁₂ NiO ₁₀ S
AFLOW prototype label	A12BC10D_tP96_92_6b_a_5b_a-001
<i>Strukturbericht</i> designation	$H4_5$
Mineral name	retgersite
ICSD	62051
Pearson symbol	tP96
Space group number	92
Space group symbol	$P4_12_12$
AFLOW prototype command	<pre>aflow --proto=A12BC10D_tP96_92_6b_a_5b_a-001 --params=a, c/a, x₁, x₂, 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</pre>

- This structure is nearly identical to the one presented in (Hermann, 1937) as $H4_5$, but now includes the positions of the hydrogen atoms.
- This compound can also be found in the enantiomorphic space group $P4_32_12$ #98.

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	$=$	$a x_1 \hat{\mathbf{x}} + a x_1 \hat{\mathbf{y}}$	(4a)	Ni I
\mathbf{B}_2	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} - a x_1 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4a)	Ni I
\mathbf{B}_3	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + (x_1 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a (x_1 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_1 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4a)	Ni I
\mathbf{B}_4	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - (x_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a (x_1 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_1 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4a)	Ni I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$a x_2 \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}}$	(4a)	S I
\mathbf{B}_6	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4a)	S I
\mathbf{B}_7	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a (x_2 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4a)	S I
\mathbf{B}_8	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a (x_2 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4a)	S I
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + a y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(8b)	H I
\mathbf{B}_{10}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - a y_3 \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	H I
\mathbf{B}_{11}	$= -(y_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-a (y_3 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_3 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_3 + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	H I
\mathbf{B}_{12}	$= (y_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{3}{4}) \mathbf{a}_3$	$=$	$a (y_3 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_3 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_3 + \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	H I
\mathbf{B}_{13}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{4}) \mathbf{a}_3$	$=$	$-a (x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c (z_3 - \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	H I
\mathbf{B}_{14}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{3}{4}) \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_3 - \frac{1}{2}) \hat{\mathbf{y}} - c (z_3 - \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	H I
\mathbf{B}_{15}	$= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a y_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(8b)	H I
\mathbf{B}_{16}	$= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a y_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	H I
\mathbf{B}_{17}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + a y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(8b)	H II
\mathbf{B}_{18}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - a y_4 \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	H II
\mathbf{B}_{19}	$= -(y_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-a (y_4 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_4 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_4 + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	H II
\mathbf{B}_{20}	$= (y_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{3}{4}) \mathbf{a}_3$	$=$	$a (y_4 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_4 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_4 + \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	H II
\mathbf{B}_{21}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{4}) \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c (z_4 - \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	H II
\mathbf{B}_{22}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{3}{4}) \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_4 - \frac{1}{2}) \hat{\mathbf{y}} - c (z_4 - \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	H II
\mathbf{B}_{23}	$= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a y_4 \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}} - c z_4 \hat{\mathbf{z}}$	(8b)	H II
\mathbf{B}_{24}	$= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a y_4 \hat{\mathbf{x}} - a x_4 \hat{\mathbf{y}} - c (z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	H II
\mathbf{B}_{25}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} + a y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(8b)	H III

$$\begin{aligned}
\mathbf{B}_{85} &= -\begin{pmatrix} x_{12} - \frac{1}{2} \\ z_{12} - \frac{1}{4} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_{12} + \frac{1}{2} \\ z_{12} - \frac{1}{4} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} \\ z_{12} - \frac{1}{4} \end{pmatrix} \mathbf{a}_3 &= & -a \begin{pmatrix} x_{12} - \frac{1}{2} \\ z_{12} - \frac{1}{4} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} y_{12} + \frac{1}{2} \\ z_{12} - \frac{1}{4} \end{pmatrix} \hat{\mathbf{y}} - c \begin{pmatrix} \\ z_{12} - \frac{1}{4} \end{pmatrix} \hat{\mathbf{z}} & (8b) & \text{O IV} \\
\mathbf{B}_{86} &= \begin{pmatrix} x_{12} + \frac{1}{2} \\ z_{12} - \frac{3}{4} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_{12} - \frac{1}{2} \\ z_{12} - \frac{3}{4} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} \\ z_{12} - \frac{3}{4} \end{pmatrix} \mathbf{a}_3 &= & a \begin{pmatrix} x_{12} + \frac{1}{2} \\ z_{12} - \frac{3}{4} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} y_{12} - \frac{1}{2} \\ z_{12} - \frac{3}{4} \end{pmatrix} \hat{\mathbf{y}} - c \begin{pmatrix} \\ z_{12} - \frac{3}{4} \end{pmatrix} \hat{\mathbf{z}} & (8b) & \text{O IV} \\
\mathbf{B}_{87} &= y_{12} \mathbf{a}_1 + x_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3 &= & ay_{12} \hat{\mathbf{x}} + ax_{12} \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}} & (8b) & \text{O IV} \\
\mathbf{B}_{88} &= -y_{12} \mathbf{a}_1 - x_{12} \mathbf{a}_2 - \begin{pmatrix} z_{12} - \frac{1}{2} \\ \\ \end{pmatrix} \mathbf{a}_3 &= & -ay_{12} \hat{\mathbf{x}} - ax_{12} \hat{\mathbf{y}} - c \begin{pmatrix} z_{12} - \frac{1}{2} \\ \\ \end{pmatrix} \hat{\mathbf{z}} & (8b) & \text{O IV} \\
\mathbf{B}_{89} &= x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3 &= & ax_{13} \hat{\mathbf{x}} + ay_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (8b) & \text{O V} \\
\mathbf{B}_{90} &= -x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 + \begin{pmatrix} z_{13} + \frac{1}{2} \\ \\ \end{pmatrix} \mathbf{a}_3 &= & -ax_{13} \hat{\mathbf{x}} - ay_{13} \hat{\mathbf{y}} + c \begin{pmatrix} z_{13} + \frac{1}{2} \\ \\ \end{pmatrix} \hat{\mathbf{z}} & (8b) & \text{O V} \\
\mathbf{B}_{91} &= -\begin{pmatrix} y_{13} - \frac{1}{2} \\ z_{13} + \frac{1}{4} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_{13} + \frac{1}{2} \\ z_{13} + \frac{1}{4} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \\ z_{13} + \frac{1}{4} \end{pmatrix} \mathbf{a}_3 &= & -a \begin{pmatrix} y_{13} - \frac{1}{2} \\ z_{13} + \frac{1}{4} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} x_{13} + \frac{1}{2} \\ z_{13} + \frac{1}{4} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} \\ z_{13} + \frac{1}{4} \end{pmatrix} \hat{\mathbf{z}} & (8b) & \text{O V} \\
\mathbf{B}_{92} &= \begin{pmatrix} y_{13} + \frac{1}{2} \\ z_{13} + \frac{3}{4} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_{13} - \frac{1}{2} \\ z_{13} + \frac{3}{4} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} \\ z_{13} + \frac{3}{4} \end{pmatrix} \mathbf{a}_3 &= & a \begin{pmatrix} y_{13} + \frac{1}{2} \\ z_{13} + \frac{3}{4} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} x_{13} - \frac{1}{2} \\ z_{13} + \frac{3}{4} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} \\ z_{13} + \frac{3}{4} \end{pmatrix} \hat{\mathbf{z}} & (8b) & \text{O V} \\
\mathbf{B}_{93} &= -\begin{pmatrix} x_{13} - \frac{1}{2} \\ z_{13} - \frac{1}{4} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_{13} + \frac{1}{2} \\ z_{13} - \frac{1}{4} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} \\ z_{13} - \frac{1}{4} \end{pmatrix} \mathbf{a}_3 &= & -a \begin{pmatrix} x_{13} - \frac{1}{2} \\ z_{13} - \frac{1}{4} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} y_{13} + \frac{1}{2} \\ z_{13} - \frac{1}{4} \end{pmatrix} \hat{\mathbf{y}} - c \begin{pmatrix} \\ z_{13} - \frac{1}{4} \end{pmatrix} \hat{\mathbf{z}} & (8b) & \text{O V} \\
\mathbf{B}_{94} &= \begin{pmatrix} x_{13} + \frac{1}{2} \\ z_{13} - \frac{3}{4} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_{13} - \frac{1}{2} \\ z_{13} - \frac{3}{4} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} \\ z_{13} - \frac{3}{4} \end{pmatrix} \mathbf{a}_3 &= & a \begin{pmatrix} x_{13} + \frac{1}{2} \\ z_{13} - \frac{3}{4} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} y_{13} - \frac{1}{2} \\ z_{13} - \frac{3}{4} \end{pmatrix} \hat{\mathbf{y}} - c \begin{pmatrix} \\ z_{13} - \frac{3}{4} \end{pmatrix} \hat{\mathbf{z}} & (8b) & \text{O V} \\
\mathbf{B}_{95} &= y_{13} \mathbf{a}_1 + x_{13} \mathbf{a}_2 - z_{13} \mathbf{a}_3 &= & ay_{13} \hat{\mathbf{x}} + ax_{13} \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}} & (8b) & \text{O V} \\
\mathbf{B}_{96} &= -y_{13} \mathbf{a}_1 - x_{13} \mathbf{a}_2 - \begin{pmatrix} z_{13} - \frac{1}{2} \\ \\ \end{pmatrix} \mathbf{a}_3 &= & -ay_{13} \hat{\mathbf{x}} - ax_{13} \hat{\mathbf{y}} - c \begin{pmatrix} z_{13} - \frac{1}{2} \\ \\ \end{pmatrix} \hat{\mathbf{z}} & (8b) & \text{O V}
\end{aligned}$$

References

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