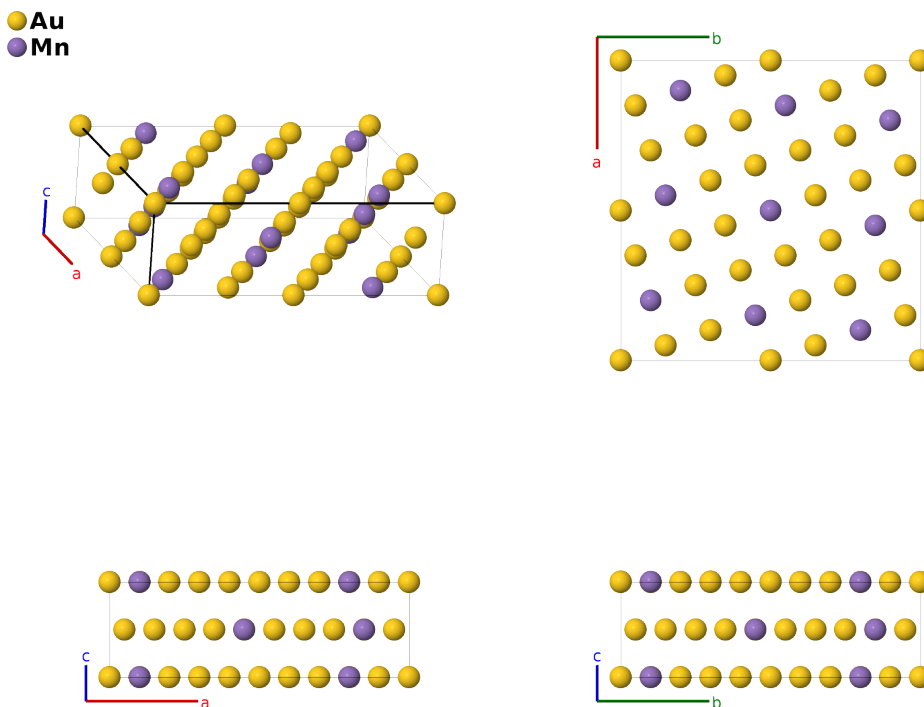


Au₃₁Mn₉ Structure: A31B9_tP40_83_ae3j4k_cjk-001

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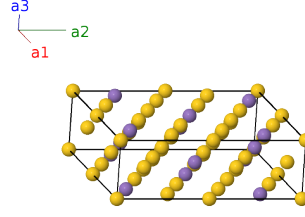
<https://aflow.org/p/FCR5>

https://aflow.org/p/A31B9_tP40_83_ae3j4k_cjk-001



Prototype	Au ₃₁ Mn ₉
AFLOW prototype label	A31B9_tP40_83_ae3j4k_cjk-001
ICSD	58552
Pearson symbol	tP40
Space group number	83
Space group symbol	<i>P4/m</i>
AFLOW prototype command	<code>aflow --proto=A31B9_tP40_83_ae3j4k_cjk-001 --params=a, c/a, x₄, y₄, x₅, y₅, x₆, y₆, x₇, y₇, x₈, y₈, x₉, y₉, x₁₀, y₁₀, x₁₁, y₁₁, x₁₂, y₁₂</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	0	$=$	0	(1a)	Au I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(1c)	Mn I
\mathbf{B}_3	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{y}}$	(2e)	Au II
\mathbf{B}_4	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(2e)	Au II
\mathbf{B}_5	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}}$	(4j)	Au III
\mathbf{B}_6	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}}$	(4j)	Au III
\mathbf{B}_7	$-y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2$	$=$	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}}$	(4j)	Au III
\mathbf{B}_8	$y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}}$	(4j)	Au III
\mathbf{B}_9	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}}$	(4j)	Au IV
\mathbf{B}_{10}	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}}$	(4j)	Au IV
\mathbf{B}_{11}	$-y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2$	$=$	$-ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}}$	(4j)	Au IV
\mathbf{B}_{12}	$y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2$	$=$	$ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}}$	(4j)	Au IV
\mathbf{B}_{13}	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2$	$=$	$ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}}$	(4j)	Au V
\mathbf{B}_{14}	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2$	$=$	$-ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}}$	(4j)	Au V
\mathbf{B}_{15}	$-y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2$	$=$	$-ay_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}}$	(4j)	Au V
\mathbf{B}_{16}	$y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2$	$=$	$ay_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}}$	(4j)	Au V
\mathbf{B}_{17}	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2$	$=$	$ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}}$	(4j)	Mn II
\mathbf{B}_{18}	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2$	$=$	$-ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}}$	(4j)	Mn II
\mathbf{B}_{19}	$-y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2$	$=$	$-ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}}$	(4j)	Mn II
\mathbf{B}_{20}	$y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2$	$=$	$ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}}$	(4j)	Mn II
\mathbf{B}_{21}	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4k)	Au VI
\mathbf{B}_{22}	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4k)	Au VI
\mathbf{B}_{23}	$-y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ay_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4k)	Au VI
\mathbf{B}_{24}	$y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ay_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4k)	Au VI
\mathbf{B}_{25}	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4k)	Au VII
\mathbf{B}_{26}	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - ay_9 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4k)	Au VII
\mathbf{B}_{27}	$-y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ay_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4k)	Au VII
\mathbf{B}_{28}	$y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ay_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4k)	Au VII
\mathbf{B}_{29}	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + ay_{10} \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4k)	Au VIII
\mathbf{B}_{30}	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} - ay_{10} \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4k)	Au VIII

$$\begin{aligned}
\mathbf{B}_{31} &= -y_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & -ay_{10} \hat{\mathbf{x}} + ax_{10} \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4k) & \text{Au VIII} \\
\mathbf{B}_{32} &= y_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & ay_{10} \hat{\mathbf{x}} - ax_{10} \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4k) & \text{Au VIII} \\
\mathbf{B}_{33} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & ax_{11} \hat{\mathbf{x}} + ay_{11} \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4k) & \text{Au IX} \\
\mathbf{B}_{34} &= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & -ax_{11} \hat{\mathbf{x}} - ay_{11} \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4k) & \text{Au IX} \\
\mathbf{B}_{35} &= -y_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & -ay_{11} \hat{\mathbf{x}} + ax_{11} \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4k) & \text{Au IX} \\
\mathbf{B}_{36} &= y_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & ay_{11} \hat{\mathbf{x}} - ax_{11} \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4k) & \text{Au IX} \\
\mathbf{B}_{37} &= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & ax_{12} \hat{\mathbf{x}} + ay_{12} \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4k) & \text{Mn III} \\
\mathbf{B}_{38} &= -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & -ax_{12} \hat{\mathbf{x}} - ay_{12} \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4k) & \text{Mn III} \\
\mathbf{B}_{39} &= -y_{12} \mathbf{a}_1 + x_{12} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & -ay_{12} \hat{\mathbf{x}} + ax_{12} \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4k) & \text{Mn III} \\
\mathbf{B}_{40} &= y_{12} \mathbf{a}_1 - x_{12} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & ay_{12} \hat{\mathbf{x}} - ax_{12} \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4k) & \text{Mn III}
\end{aligned}$$

References

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