$Au_{31}Mn_9$ Structure: A31B9_tP40_83_ae3j4k_cjk-001

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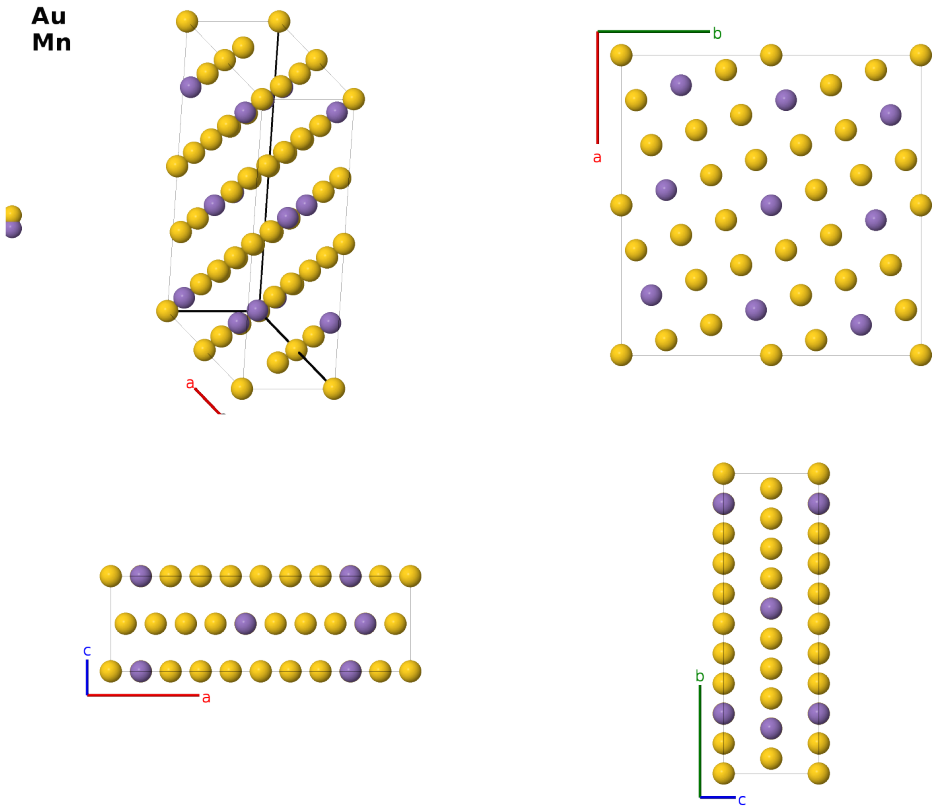
https://aflow.org/prototype-encyclopedia/FCR5

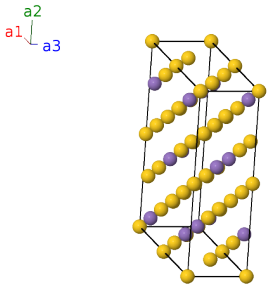
https://aflow.org/prototype-encyclopedia/A31B9_tP40_83_ae3j4k_cjk-001



Prototype	$Au_{31}Mn_9$
AFLOW prototype label	A31B9_tP40_83_ae3j4k_cjk-001
ICSD	58552
CCDC	1622563
Pearson symbol	tP40
Space group number	83
Space group symbol	$P4/m$
AFLOW prototype command	`aflow --proto=A31B9_tP40_83_ae3j4k_cjk-001 --params=`$a, c/a, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7, x_8, y_8, x_9, y_9, x_{10}, y_{10}, x_{11}, y_{11}, x_{12}, y_{12}$

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
$\mathbf{B_{31}}$	=	$-y_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ay_{10}\,\hat{\mathbf{x}} + ax_{10}\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4k)	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)	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)	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)	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)	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)	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)	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)	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)	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)	Mn III

References

[1] K. Hiraga, D. Shindo, M. Hirabayashi, O. Terasaki, and D. Watanabe, *A study of the ordered structures of the Au-Mn system by high-voltage-high-resolution electron microscopy. I. Two-dimensional antiphase structure of $Au_{31}Mn_9$ based on the Au_4Mn structure*, Acta Crystallogr. Sect. B **36**, 2550–2554 (1980), doi:10.1107/S0567740880009417.

Found in

[1] `http://icsd.fiz-karlsruhe.de/`. ICSD Entry 150552.

First cited in

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