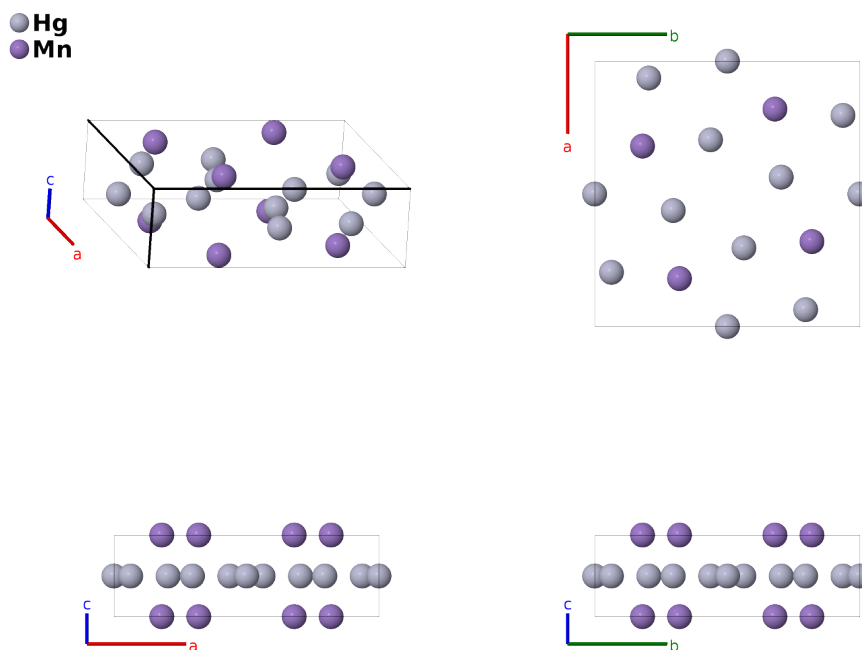


# Mn<sub>2</sub>Hg<sub>5</sub> Structure: A5B2\_tP14\_127\_cj\_g-001

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

[https://aflow.org/p/A5B2\\_tP14\\_127\\_cj\\_g-001](https://aflow.org/p/A5B2_tP14_127_cj_g-001)



Prototype	Hg <sub>5</sub> Mn <sub>2</sub>
AFLOW prototype label	A5B2_tP14_127_cj_g-001
ICSD	104324
Pearson symbol	tP14
Space group number	127
Space group symbol	<i>P4/mbm</i>
AFLOW prototype command	<code>aflow --proto=A5B2_tP14_127_cj_g-001 --params=a, c/a, x<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub></code>

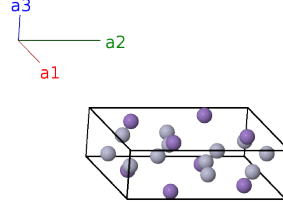
## Other compounds with this structure

Ag<sub>2</sub>Hg<sub>5</sub>, Hf<sub>2</sub>In<sub>5</sub>, Li<sub>2</sub>Sn<sub>5</sub>, Mn<sub>2</sub>Ga<sub>5</sub>, Pd<sub>2</sub>Hg<sub>5</sub>, Ti<sub>2</sub>In<sub>5</sub>, V<sub>2</sub>Ga<sub>5</sub>, W<sub>2</sub>Ga<sub>5</sub>, Ti<sub>3</sub>In<sub>4</sub>

- We shifted the origin of the *c*-axis by *c*/2 from that used by (de Wet, 1961).

## 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
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2c)	Hg I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2c)	Hg I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Mn I
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Mn I
$\mathbf{B}_5$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(4g)	Mn I
$\mathbf{B}_6$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}}$	(4g)	Mn I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	Hg II
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	Hg II
$\mathbf{B}_9$	$= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	Hg II
$\mathbf{B}_{10}$	$= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	Hg II
$\mathbf{B}_{11}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	Hg II
$\mathbf{B}_{12}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	Hg II
$\mathbf{B}_{13}$	$= (y_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	Hg II
$\mathbf{B}_{14}$	$= -(y_3 - \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	Hg II

## References

- [1] J. F. de Wet, *The Crystal Structure of  $Mn_2Hg_5$* , *Acta Cryst.* **14**, 733–738 (1961), doi:10.1107/S0365110X61002229.

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