# $Mn_2Hg_5$ Structure: A5B2_tP14_127_cj_g-001

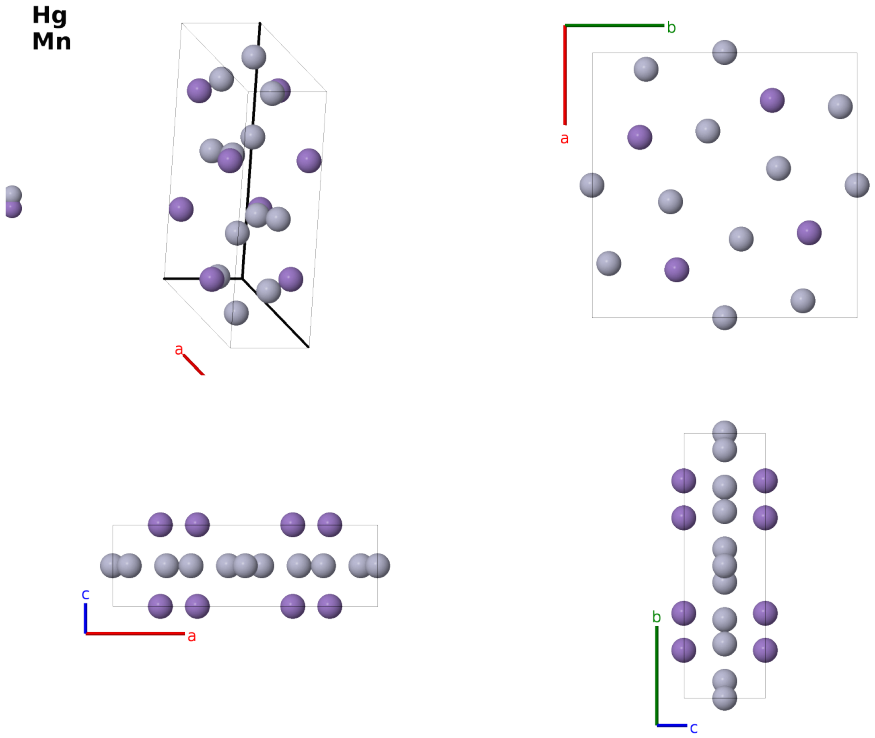
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

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

https://aflow.org/prototype-encyclopedia/A5B2_tP14_127_cj_g-001




| | |
|---|---|
| **Prototype** | $Hg_5Mn_2$ |
| **AFLOW prototype label** | A5B2_tP14_127_cj_g-001 |
| **ICSD** | 104324 |
| **CCDC** | 1662240 |
| **Pearson symbol** | tP14 |
| **Space group number** | 127 |
| **Space group symbol** | $P4/mbm$ |
| **AFLOW prototype command** | `aflow --proto=A5B2_tP14_127_cj_g-001 --params=`$a, c/a, x_2, x_3, y_3$ |

---

**Other compounds with this structure**

$Ag_2Hg_5$, $Hf_2In_5$, $Li_2Sn_5$, $Mn_2Ga_5$, $Pd_2Hg_5$, $Ti_2In_5$, $V_2Ga_5$, $W_2Ga_5$, $Ti_3In_4$

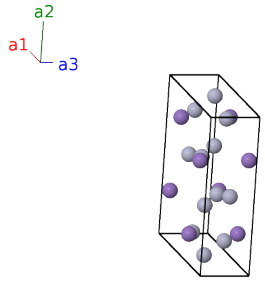
---

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

---

**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 |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (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 |
| $\mathbf{B_3}$ | = | $x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2$ | = | $ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$ | (4g) | Mn I |
| $\mathbf{B_4}$ | = | $-x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2$ | = | $-ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$ | (4g) | Mn I |
| $\mathbf{B_5}$ | = | $-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$ | = | $-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$ | (4g) | Mn I |
| $\mathbf{B_6}$ | = | $\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$ | = | $a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$ | (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 |
| $\mathbf{B_{11}}$ | = | $-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (8j) | Hg II |
| $\mathbf{B_{12}}$ | = | $\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (8j) | Hg II |
| $\mathbf{B_{13}}$ | = | $\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (8j) | Hg II |
| $\mathbf{B_{14}}$ | = | $-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (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.


**Found in**


[1] V. J. Yannello, E. Lu, and D. C. Fredrickson, *At the Limits of Isolobal Bonding: $\pi$-Based Covalent Magnetism in $Mn_2Hg_5$*, Inorg. Chem. **59**, 12304–12313 (2020), doi:10.1021/acs.inorgchem.0c01393.


**First cited in**


H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.