

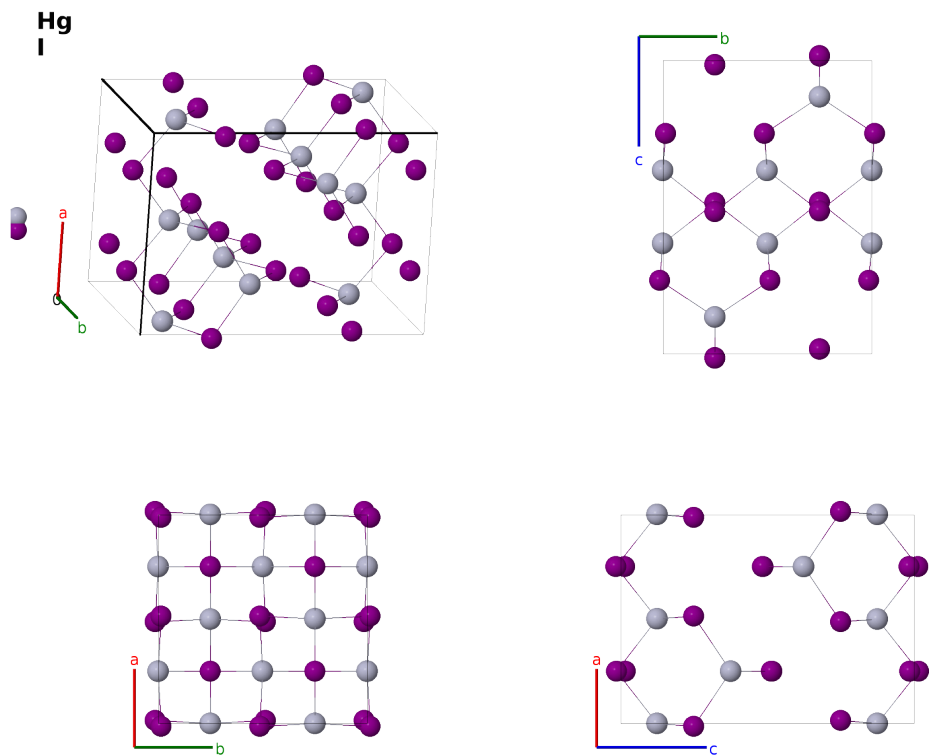
Orange (II) HgI₂ Structure: AB2_tP24_137_g_cdf-001

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/L566>

https://aflow.org/prototype-encyclopedia/AB2_tP24_137_g_cdf-001



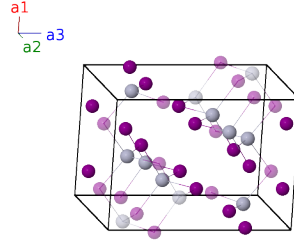
Prototype	HgI ₂
AFLOW prototype label	AB2_tP24_137_g_cdf-001
ICSD	281133
CCDC	1721725
Pearson symbol	tP24
Space group number	137
Space group symbol	$P4_2/nmc$
AFLOW prototype command	<code>aflow --proto=AB2_tP24_137_g_cdf-001</code> <code>--params=$a, c/a, z_1, z_2, x_3, y_4, z_4$</code>

- HgI_2 can be found in a variety of forms (Gumiński, 1997):

- The ground state, coccinite, also known as red or $\alpha\text{-HgI}_2$ and given the *Strukturbericht* designation *C13*. It is stable up to 135°C .
- At higher temperatures this transforms into yellow or $\beta\text{-HgI}_2$ in the HgBr_2 (*C24*) structure. This is stable up to the melting point at 258°C .
- (Schwarzenbach, 1969) studied the metastable orange HgI_2 body-centered tetragonal ($I4_1/amd$ #141) phase. This structure was refined by (Hostettler, 2002).
- (Hostettler, 2002) also found a second orange HgI_2 phase (this structure) in a simple tetragonal ($P4_2/nmc$ #137) cell.
- The last two structures differ by stacking order. (Hostettler, 2002) used them to produce an averaged orange HgI_2 structure, space group $P4m2$ #115.

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
$\mathbf{B}_1$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	I I
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	I I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	I I
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	I I
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4d)	I II
$\mathbf{B}_6$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	I II
$\mathbf{B}_7$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4d)	I II
$\mathbf{B}_8$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	I II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8f)	I III
$\mathbf{B}_{10}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8f)	I III
$\mathbf{B}_{11}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8f)	I III
$\mathbf{B}_{12}$	$= -x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8f)	I III
$\mathbf{B}_{13}$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8f)	I III
$\mathbf{B}_{14}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8f)	I III
$\mathbf{B}_{15}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8f)	I III
$\mathbf{B}_{16}$	$= x_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8f)	I III
$\mathbf{B}_{17}$	$= \frac{1}{4} \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	Hg I
$\mathbf{B}_{18}$	$= \frac{1}{4} \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	Hg I

$$\begin{aligned}
\mathbf{B}_{19} &= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8g) &\text{Hg I} \\
\mathbf{B}_{20} &= y_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 &= ay_4 \hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8g) &\text{Hg I} \\
\mathbf{B}_{21} &= \frac{3}{4} \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \frac{3}{4}a\hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} &(8g) &\text{Hg I} \\
\mathbf{B}_{22} &= \frac{3}{4} \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \frac{3}{4}a\hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} &(8g) &\text{Hg I} \\
\mathbf{B}_{23} &= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8g) &\text{Hg I} \\
\mathbf{B}_{24} &= -y_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 &= -ay_4 \hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8g) &\text{Hg I}
\end{aligned}$$

References

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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.