Orange (I) HgI_2 Structure: AB2_tI48_141_h_2eg-001

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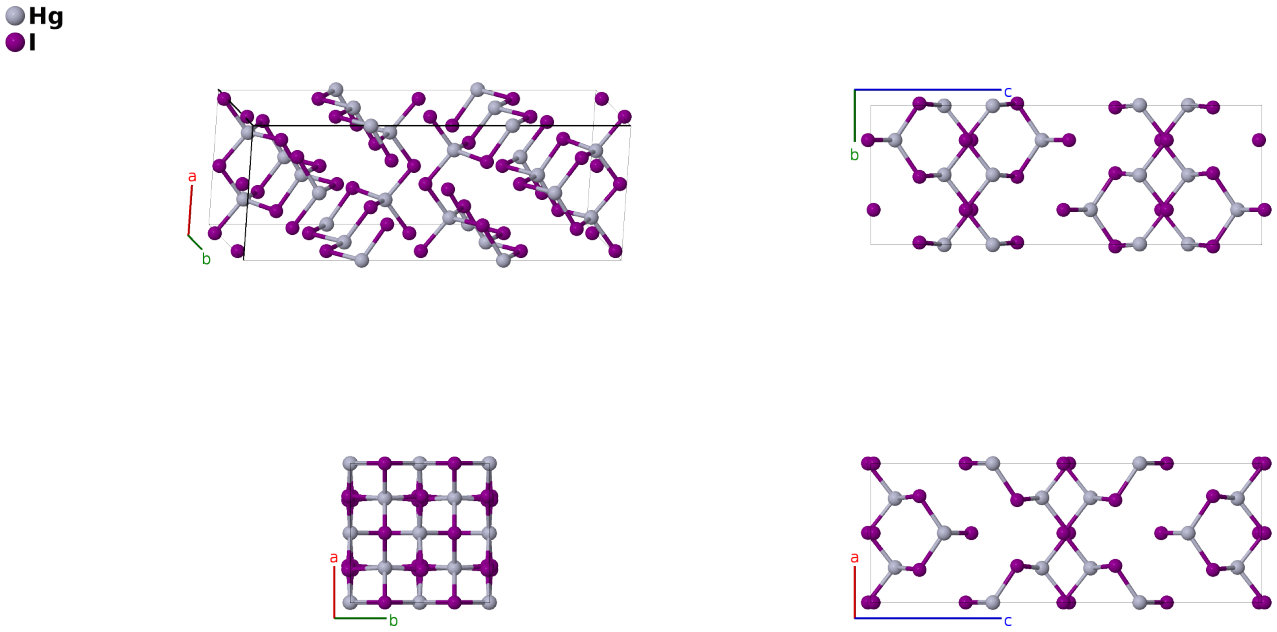
https://aflow.org/p/Q9V3

https://aflow.org/p/AB2_tI48_141_h_2eg-001



Prototype	HgI_2
AFLOW prototype label	AB2_tI48_141_h_2eg-001
ICSD	18126
Pearson symbol	tI48
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	`aflow --proto=AB2_tI48_141_h_2eg-001 --params=`$a, c/a, z_1, z_2, x_3, y_4, z_4$

- HgI_2 can be found in a variety of forms (Gumiński, 1997):
  - The ground state, coccinite, also known as red or α-HgI_2 and given the *Strukturbericht* designation $C13$. It is stable up to 135°C.
  - At higher temperatures this transforms into yellow or β-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 (this structure) body-centered tetragonal ($I4_1/amd$ #141) phase. This structure was refined by (Hostettler, 2002).

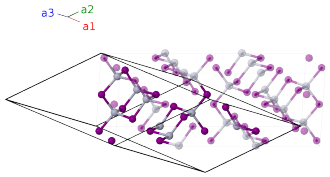
– (Hostettler, 2002) also found a second orange HgI_2 phase in a simple tetragonal ($P4_2/nmc$ #137) cell.

– The last two structures differ by stacking order. (Hostettler, 2002) used them to produce an averaged orange HgI_2 structure, space group $P\bar{4}m2$ #115.

- The ICSD entry for this structure is from the earlier work of (Schwarzenbach, 1969).

Body-centered Tetragonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\left(z_1+\frac{1}{4}\right)\mathbf{a}_1 + z_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8e)	I I
$\mathbf{B_2}$	=	$z_1\,\mathbf{a}_1 + \left(z_1+\frac{1}{4}\right)\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_1-\frac{1}{4}\right)\hat{\mathbf{z}}$	(8e)	I I
$\mathbf{B_3}$	=	$-\left(z_1-\frac{3}{4}\right)\mathbf{a}_1 - z_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8e)	I I
$\mathbf{B_4}$	=	$-z_1\,\mathbf{a}_1 - \left(z_1-\frac{3}{4}\right)\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_1-\frac{1}{4}\right)\hat{\mathbf{z}}$	(8e)	I I
$\mathbf{B_5}$	=	$\left(z_2+\frac{1}{4}\right)\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8e)	I II
$\mathbf{B_6}$	=	$z_2\,\mathbf{a}_1 + \left(z_2+\frac{1}{4}\right)\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_2-\frac{1}{4}\right)\hat{\mathbf{z}}$	(8e)	I II
$\mathbf{B_7}$	=	$-\left(z_2-\frac{3}{4}\right)\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8e)	I II
$\mathbf{B_8}$	=	$-z_2\,\mathbf{a}_1 - \left(z_2-\frac{3}{4}\right)\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_2-\frac{1}{4}\right)\hat{\mathbf{z}}$	(8e)	I II
$\mathbf{B_9}$	=	$\left(x_3+\frac{1}{8}\right)\mathbf{a}_1 + \left(x_3+\frac{7}{8}\right)\mathbf{a}_2 + \left(2x_3+\frac{1}{4}\right)\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_3-\frac{1}{4}\right)\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16g)	I III
$\mathbf{B_{10}}$	=	$-\left(x_3-\frac{1}{8}\right)\mathbf{a}_1 - \left(x_3-\frac{7}{8}\right)\mathbf{a}_2 - \left(2x_3-\frac{1}{4}\right)\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_3+\frac{1}{4}\right)\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16g)	I III
$\mathbf{B_{11}}$	=	$\left(x_3+\frac{7}{8}\right)\mathbf{a}_1 - \left(x_3-\frac{1}{8}\right)\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + a\left(x_3+\frac{3}{4}\right)\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16g)	I III
$\mathbf{B_{12}}$	=	$-\left(x_3-\frac{7}{8}\right)\mathbf{a}_1 + \left(x_3+\frac{1}{8}\right)\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - a\left(x_3-\frac{3}{4}\right)\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16g)	I III
$\mathbf{B_{13}}$	=	$-\left(x_3-\frac{7}{8}\right)\mathbf{a}_1 - \left(x_3-\frac{1}{8}\right)\mathbf{a}_2 - \left(2x_3-\frac{3}{4}\right)\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3-\frac{3}{4}\right)\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16g)	I III
$\mathbf{B_{14}}$	=	$\left(x_3+\frac{7}{8}\right)\mathbf{a}_1 + \left(x_3+\frac{1}{8}\right)\mathbf{a}_2 + \left(2x_3+\frac{3}{4}\right)\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3+\frac{3}{4}\right)\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16g)	I III
$\mathbf{B_{15}}$	=	$-\left(x_3-\frac{1}{8}\right)\mathbf{a}_1 + \left(x_3+\frac{7}{8}\right)\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_3+\frac{1}{4}\right)\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16g)	I III
$\mathbf{B_{16}}$	=	$\left(x_3+\frac{1}{8}\right)\mathbf{a}_1 - \left(x_3-\frac{7}{8}\right)\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_3-\frac{1}{4}\right)\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16g)	I III
$\mathbf{B_{17}}$	=	$\left(y_4+z_4\right)\mathbf{a}_1 + z_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16h)	Hg I
$\mathbf{B_{18}}$	=	$\left(-y_4+z_4+\frac{1}{2}\right)\mathbf{a}_1 + z_4\,\mathbf{a}_2 - \left(y_4-\frac{1}{2}\right)\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{2}\right)\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16h)	Hg I
$\mathbf{B_{19}}$	=	$z_4\,\mathbf{a}_1 + \left(-y_4+z_4+\frac{1}{2}\right)\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{4}\right)\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16h)	Hg I
$\mathbf{B_{20}}$	=	$z_4\,\mathbf{a}_1 + \left(y_4+z_4\right)\mathbf{a}_2 + \left(y_4+\frac{1}{2}\right)\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{4}\right)\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_4-\frac{1}{4}\right)\hat{\mathbf{z}}$	(16h)	Hg I
$\mathbf{B_{21}}$	=	$\left(y_4-z_4+\frac{1}{2}\right)\mathbf{a}_1 - z_4\,\mathbf{a}_2 + \left(y_4+\frac{1}{2}\right)\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{2}\right)\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16h)	Hg I
$\mathbf{B_{22}}$	=	$-\left(y_4+z_4\right)\mathbf{a}_1 - z_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16h)	Hg I

$\mathbf{B_{23}}$	=	$-z_4\,\mathbf{a}_1+\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_2+y_4\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{4}\right)\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	Hg I
$\mathbf{B_{24}}$	=	$-z_4\,\mathbf{a}_1-(y_4+z_4)\,\mathbf{a}_2-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	Hg I