Orange (I) HgI_2 Structure: AB2_tI48_141_h_2eg-001

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https://aflow.org/prototype-encyclopedia/Q9V3

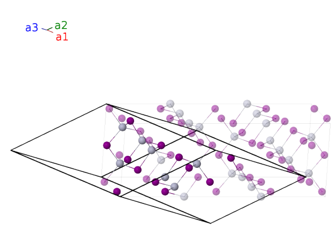
https://aflow.org/prototype-encyclopedia/AB2_tI48_141_h_2eg-001

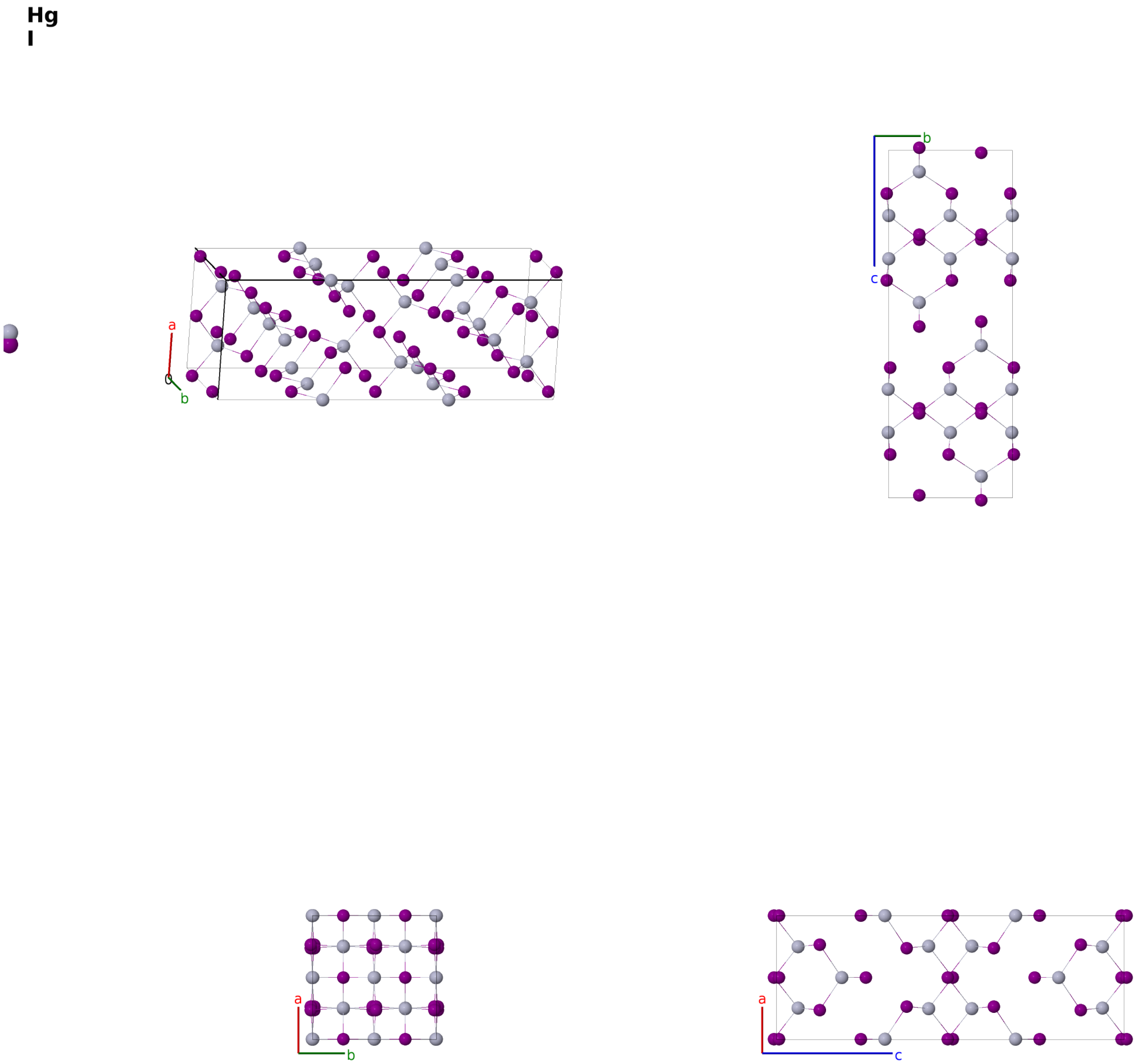
Prototype	HgI_2
AFLOW prototype label	AB2_tI48_141_h_2eg-001
ICSD	18126
CCDC	1597683
Pearson symbol	tI48
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	`aflow --proto=AB2_tI48_141_h_2eg-001 --params=`$a, c/a, z_1, z_2, x_3, y_4, z_4$

- 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

$$\mathbf{a_1} = -\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - \frac{1}{2}c\,\hat{\mathbf{z}}$$




Hg
I
a
b
c

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_{1}}$	=	$\left(z_{1}+\frac{1}{4}\right)\,\mathbf{a}_{1}+z_{1}\,\mathbf{a}_{2}+\frac{1}{4}\,\mathbf{a}_{3}$	=	$\frac{1}{4}a\,\mathbf{\hat{y}}+cz_{1}\,\mathbf{\hat{z}}$	(8e)	I I
$\mathbf{B_{2}}$	=	$z_{1}\,\mathbf{a}_{1}+\left(z_{1}+\frac{1}{4}\right)\,\mathbf{a}_{2}+\frac{3}{4}\,\mathbf{a}_{3}$	=	$\frac{1}{2}a\,\mathbf{\hat{x}}+\frac{1}{4}a\,\mathbf{\hat{y}}+c\left(z_{1}-\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(8e)	I I
$\mathbf{B_{3}}$	=	$-\left(z_{1}-\frac{3}{4}\right)\,\mathbf{a}_{1}-z_{1}\,\mathbf{a}_{2}+\frac{3}{4}\,\mathbf{a}_{3}$	=	$\frac{3}{4}a\,\mathbf{\hat{y}}-cz_{1}\,\mathbf{\hat{z}}$	(8e)	I I
$\mathbf{B_{4}}$	=	$-z_{1}\,\mathbf{a}_{1}-\left(z_{1}-\frac{3}{4}\right)\,\mathbf{a}_{2}+\frac{1}{4}\,\mathbf{a}_{3}$	=	$\frac{1}{2}a\,\mathbf{\hat{x}}-\frac{1}{4}a\,\mathbf{\hat{y}}-c\left(z_{1}-\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(8e)	I I
$\mathbf{B_{5}}$	=	$\left(z_{2}+\frac{1}{4}\right)\,\mathbf{a}_{1}+z_{2}\,\mathbf{a}_{2}+\frac{1}{4}\,\mathbf{a}_{3}$	=	$\frac{1}{4}a\,\mathbf{\hat{y}}+cz_{2}\,\mathbf{\hat{z}}$	(8e)	I II
$\mathbf{B_{6}}$	=	$z_{2}\,\mathbf{a}_{1}+\left(z_{2}+\frac{1}{4}\right)\,\mathbf{a}_{2}+\frac{3}{4}\,\mathbf{a}_{3}$	=	$\frac{1}{2}a\,\mathbf{\hat{x}}+\frac{1}{4}a\,\mathbf{\hat{y}}+c\left(z_{2}-\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(8e)	I II
$\mathbf{B_{7}}$	=	$-\left(z_{2}-\frac{3}{4}\right)\,\mathbf{a}_{1}-z_{2}\,\mathbf{a}_{2}+\frac{3}{4}\,\mathbf{a}_{3}$	=	$\frac{3}{4}a\,\mathbf{\hat{y}}-cz_{2}\,\mathbf{\hat{z}}$	(8e)	I II
$\mathbf{B_{8}}$	=	$-z_{2}\,\mathbf{a}_{1}-\left(z_{2}-\frac{3}{4}\right)\,\mathbf{a}_{2}+\frac{1}{4}\,\mathbf{a}_{3}$	=	$\frac{1}{2}a\,\mathbf{\hat{x}}-\frac{1}{4}a\,\mathbf{\hat{y}}-c\left(z_{2}-\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(8e)	I II
$\mathbf{B_{9}}$	=	$\left(x_{3}+\frac{1}{8}\right)\,\mathbf{a}_{1}+\left(x_{3}+\frac{7}{8}\right)\,\mathbf{a}_{2}+\left(2x_{3}+\frac{1}{4}\right)\,\mathbf{a}_{3}$	=	$a\left(x_{3}+\frac{1}{2}\right)\,\mathbf{\hat{x}}+a\left(x_{3}-\frac{1}{4}\right)\,\mathbf{\hat{y}}+\frac{3}{8}c\,\mathbf{\hat{z}}$	(16g)	I III
$\mathbf{B_{10}}$	=	$-\left(x_{3}-\frac{1}{8}\right)\,\mathbf{a}_{1}-\left(x_{3}-\frac{7}{8}\right)\,\mathbf{a}_{2}-\left(2x_{3}-\frac{1}{4}\right)\,\mathbf{a}_{3}$	=	$-a\left(x_{3}-\frac{1}{2}\right)\,\mathbf{\hat{x}}-a\left(x_{3}+\frac{1}{4}\right)\,\mathbf{\hat{y}}+\frac{3}{8}c\,\mathbf{\hat{z}}$	(16g)	I III
$\mathbf{B_{11}}$	=	$\left(x_{3}+\frac{7}{8}\right)\,\mathbf{a}_{1}-\left(x_{3}-\frac{1}{8}\right)\,\mathbf{a}_{2}+\frac{3}{4}\,\mathbf{a}_{3}$	=	$-ax_{3}\,\mathbf{\hat{x}}+a\left(x_{3}+\frac{3}{4}\right)\,\mathbf{\hat{y}}+\frac{1}{8}c\,\mathbf{\hat{z}}$	(16g)	I III
$\mathbf{B_{12}}$	=	$-\left(x_{3}-\frac{7}{8}\right)\,\mathbf{a}_{1}+\left(x_{3}+\frac{1}{8}\right)\,\mathbf{a}_{2}+\frac{3}{4}\,\mathbf{a}_{3}$	=	$ax_{3}\,\mathbf{\hat{x}}-a\left(x_{3}-\frac{3}{4}\right)\,\mathbf{\hat{y}}+\frac{1}{8}c\,\mathbf{\hat{z}}$	(16g)	I III
$\mathbf{B_{13}}$	=	$-\left(x_{3}-\frac{7}{8}\right)\,\mathbf{a}_{1}-\left(x_{3}-\frac{1}{8}\right)\,\mathbf{a}_{2}-\left(2x_{3}-\frac{3}{4}\right)\,\mathbf{a}_{3}$	=	$-ax_{3}\,\mathbf{\hat{x}}-a\left(x_{3}-\frac{3}{4}\right)\,\mathbf{\hat{y}}+\frac{1}{8}c\,\mathbf{\hat{z}}$	(16g)	I III
$\mathbf{B_{14}}$	=	$\left(x_{3}+\frac{7}{8}\right)\,\mathbf{a}_{1}+\left(x_{3}+\frac{1}{8}\right)\,\mathbf{a}_{2}+\left(2x_{3}+\frac{3}{4}\right)\,\mathbf{a}_{3}$	=	$ax_{3}\,\mathbf{\hat{x}}+a\left(x_{3}+\frac{3}{4}\right)\,\mathbf{\hat{y}}+\frac{1}{8}c\,\mathbf{\hat{z}}$	(16g)	I III
$\mathbf{B_{15}}$	=	$-\left(x_{3}-\frac{1}{8}\right)\,\mathbf{a}_{1}+\left(x_{3}+\frac{7}{8}\right)\,\mathbf{a}_{2}+\frac{1}{4}\,\mathbf{a}_{3}$	=	$a\left(x_{3}+\frac{1}{2}\right)\,\mathbf{\hat{x}}-a\left(x_{3}+\frac{1}{4}\right)\,\mathbf{\hat{y}}+\frac{3}{8}c\,\mathbf{\hat{z}}$	(16g)	I III
$\mathbf{B_{16}}$	=	$\left(x_{3}+\frac{1}{8}\right)\,\mathbf{a}_{1}-\left(x_{3}-\frac{7}{8}\right)\,\mathbf{a}_{2}+\frac{1}{4}\,\mathbf{a}_{3}$	=	$-a\left(x_{3}-\frac{1}{2}\right)\,\mathbf{\hat{x}}+a\left(x_{3}-\frac{1}{4}\right)\,\mathbf{\hat{y}}+\frac{3}{8}c\,\mathbf{\hat{z}}$	(16g)	I III
$\mathbf{B_{17}}$	=	$\left(y_{4}+z_{4}\right)\,\mathbf{a}_{1}+z_{4}\,\mathbf{a}_{2}+y_{4}\,\mathbf{a}_{3}$	=	$ay_{4}\,\mathbf{\hat{y}}+cz_{4}\,\mathbf{\hat{z}}$	(16h)	Hg I
$\mathbf{B_{18}}$	=	$\left(-y_{4}+z_{4}+\frac{1}{2}\right)\,\mathbf{a}_{1}+z_{4}\,\mathbf{a}_{2}-\left(y_{4}-\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-a\left(y_{4}-\frac{1}{2}\right)\,\mathbf{\hat{y}}+cz_{4}\,\mathbf{\hat{z}}$	(16h)	Hg I
$\mathbf{B_{19}}$	=	$z_{4}\,\mathbf{a}_{1}+\left(-y_{4}+z_{4}+\frac{1}{2}\right)\,\mathbf{a}_{2}-y_{4}\,\mathbf{a}_{3}$	=	$-a\left(y_{4}-\frac{1}{4}\right)\,\mathbf{\hat{x}}-\frac{1}{4}a\,\mathbf{\hat{y}}+c\left(z_{4}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16h)	Hg I
$\mathbf{B_{20}}$	=	$z_{4}\,\mathbf{a}_{1}+\left(y_{4}+z_{4}\right)\,\mathbf{a}_{2}+\left(y_{4}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$a\left(y_{4}+\frac{1}{4}\right)\,\mathbf{\hat{x}}+\frac{1}{4}a\,\mathbf{\hat{y}}+c\left(z_{4}-\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16h)	Hg I
$\mathbf{B_{21}}$	=	$\left(y_{4}-z_{4}+\frac{1}{2}\right)\,\mathbf{a}_{1}-z_{4}\,\mathbf{a}_{2}+\left(y_{4}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$a\left(y_{4}+\frac{1}{2}\right)\,\mathbf{\hat{y}}-cz_{4}\,\mathbf{\hat{z}}$	(16h)	Hg I
$\mathbf{B_{22}}$	=	$-\left(y_{4}+z_{4}\right)\,\mathbf{a}_{1}-z_{4}\,\mathbf{a}_{2}-y_{4}\,\mathbf{a}_{3}$	=	$-ay_{4}\,\mathbf{\hat{y}}-cz_{4}\,\mathbf{\hat{z}}$	(16h)	Hg I
$\mathbf{B_{23}}$	=	$-z_{4}\,\mathbf{a}_{1}+\left(y_{4}-z_{4}+\frac{1}{2}\right)\,\mathbf{a}_{2}+y_{4}\,\mathbf{a}_{3}$	=	$a\left(y_{4}+\frac{1}{4}\right)\,\mathbf{\hat{x}}-\frac{1}{4}a\,\mathbf{\hat{y}}-c\left(z_{4}-\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16h)	Hg I
$\mathbf{B_{24}}$	=	$-z_{4}\,\mathbf{a}_{1}-\left(y_{4}+z_{4}\right)\,\mathbf{a}_{2}-\left(y_{4}-\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-a\left(y_{4}-\frac{1}{4}\right)\,\mathbf{\hat{x}}+\frac{1}{4}a\,\mathbf{\hat{y}}-c\left(z_{4}+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(16h)	Hg I

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