$E3_1$ (β-Ag_2HgI_4) Structure: A2BC4_tP7_111_e_b_n-001

This structure originally had the label `A2BC4_tP7_111_f_a_n`. Calls to that address will be redirected here.

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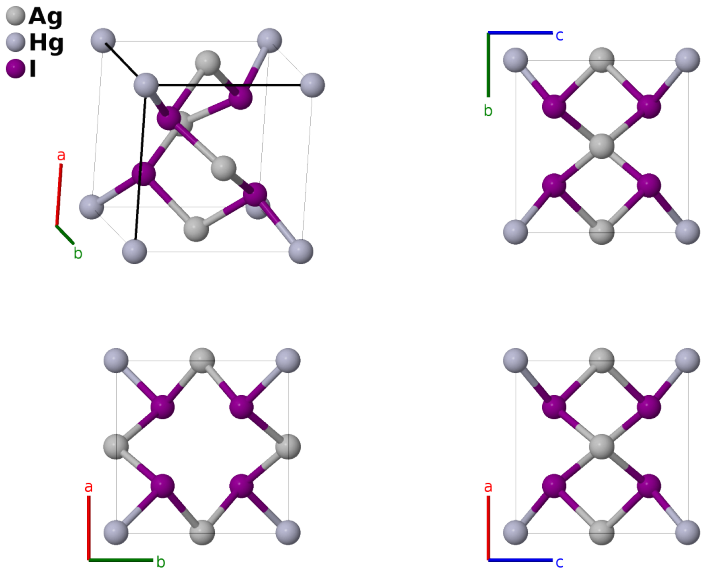
https://aflow.org/p/34W5

https://aflow.org/p/A2BC4_tP7_111_e_b_n-001



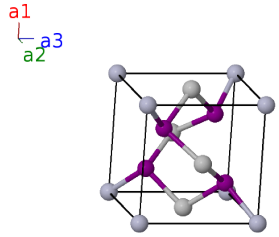
Prototype	Ag_2HgI_4
AFLOW prototype label	A2BC4_tP7_111_e_b_n-001
***Strukturbericht* designation**	$E3_1$
ICSD	30264
Pearson symbol	tP7
Space group number	111
Space group symbol	$P\bar{4}2m$
AFLOW prototype command	`aflow --proto=A2BC4_tP7_111_e_b_n-001 --params=`$a, c/a, x_3, z_3$

Other compounds with this structure
$CdIn_2Se_4$, $CuHg_2I_4$

- (Ketelaar, 1931) determined this pseudo-cubic structure for β-Ag_2HgI_4, and (Hermann, 1937) assigned it the *Strukturbericht* symbol $E3_1$. Later, (Browall, 1974) showed that β-Ag_2HgI_4 takes the Al_2CdS_4 structure, which (Pearson, 1967) listed as *Strukturbericht* $E3$.
- The $CdIn_2Se_4$ structure found by (Hahn, 1955) does seem to be in this phase, so we have removed the "obsolete" label.

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
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Hg I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2e)	Ag I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(2e)	Ag I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4n)	I I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4n)	I I
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4n)	I I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4n)	I I

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