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

This structure previously used the label(s) `A2BC4_tP7_111_f_a_n`. Calls to these addresses will be redirected here.

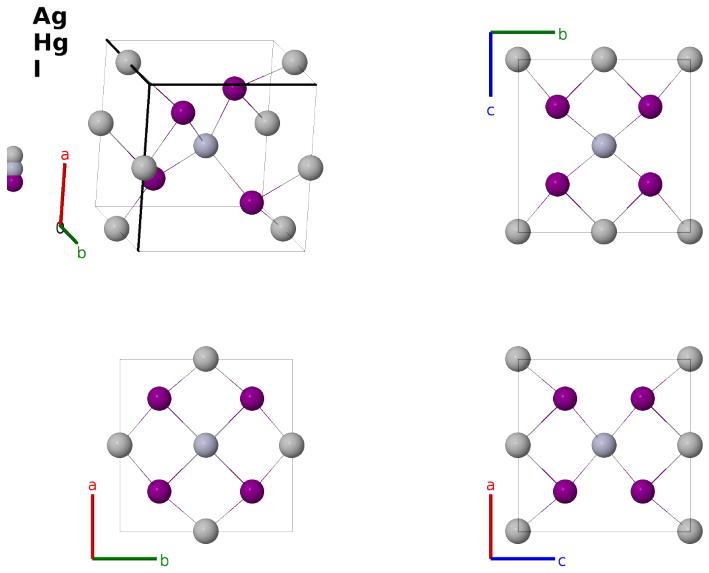
Cite this page as:

- 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/34W5

https://aflow.org/prototype-encyclopedia/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
CCDC	1604632
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=`$a, c/a, x_3, z_3$

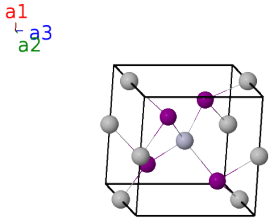
Other compounds with this structure

$CdIn_2Se_4$, $CuHg_2I_4$

- (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

References

[1] J. A. A. Ketelaar, *Strukturbestimmung der komplexen Quecksilberverbindungen Ag_2HgJ_4 und Cu_2HgJ_4*, Z. Krystallogr. **60**, 190–203 (1931), doi:10.1524/zkri.1931.80.1.190.

[2] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

[3] H. Hahn, G. Frank, W. Klingler, A. D. Störger, and G. Störger, *Untersuchungen über ternäre Chalkogenide. VI. Über Ternäre Chalkogenide des Aluminiums, Galliums und Indiums mit Zink, Cadmium und Quecksilber*, Z. Anorganische und Allgemeine Chemie **279**, 241–270 (1955), doi:10.1002/zaac.19552790502.

[4] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, Volume 2*, *International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 8 (Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1967).

Found in

[1] K. W. Browall, J. S. Kasper, and H. Wiedemeier, *Single-crystal studies of β-Ag_2HgI_4*, J. Solid State Chem. **10**, 20–28 (1974), doi:10.1016/0022-4596(74)90004-8.

First cited in

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.