$Hg_3S_2I_2$ Structure: A3B2C2_oI56_74_fhi_2ei_j-001

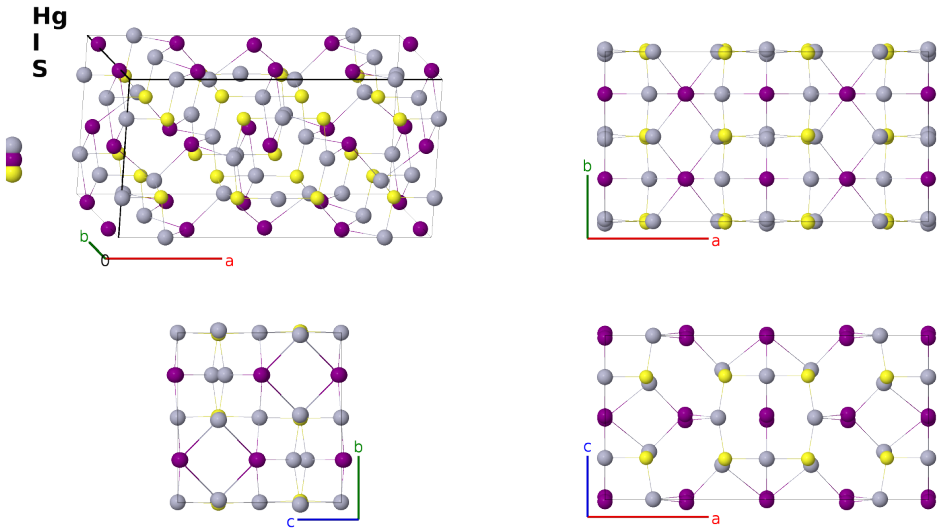
Cite this page as:

- 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/EXRV

https://aflow.org/prototype-encyclopedia/A3B2C2_oI56_74_fhi_2ei_j-001



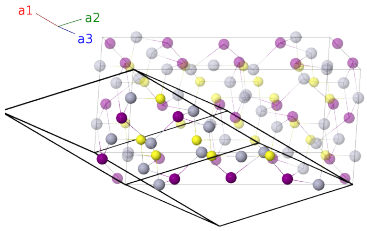
Prototype	$Hg_3I_2S_2$
AFLOW prototype label	A3B2C2_oI56_74_fhi_2ei_j-001
ICSD	411154
CCDC	1726856
Pearson symbol	oI56
Space group number	74
Space group symbol	$Imma$
AFLOW prototype command	`aflow --proto=A3B2C2_oI56_74_fhi_2ei_j-001 --params=`$a, b/a, c/a, z_1, z_2, x_3, y_4, z_4, x_5, z_5, x_6, z_6, x_7, y_7, z_7$

Other compounds with this structure
$Hg_3Se_2I_2$

- FINDSYM rotated this structure by 90° about the z-axis and shifted the origin by $(\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3)/4$ compared to the structure in (Beck, 2000).

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\left(z_1+\frac{1}{4}\right)\mathbf{a}_1 + z_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4e)	I I
$\mathbf{B_2}$	=	$-\left(z_1-\frac{3}{4}\right)\mathbf{a}_1 - z_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4e)	I I
$\mathbf{B_3}$	=	$\left(z_2+\frac{1}{4}\right)\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4e)	I II
$\mathbf{B_4}$	=	$-\left(z_2-\frac{3}{4}\right)\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4e)	I II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(8f)	Hg I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(x_3-\frac{1}{2}\right)\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(8f)	Hg I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(8f)	Hg I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(x_3+\frac{1}{2}\right)\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(8f)	Hg I
$\mathbf{B_9}$	=	$(y_4+z_4)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8h)	Hg II
$\mathbf{B_{10}}$	=	$\left(-y_4+z_4+\frac{1}{2}\right)\mathbf{a}_1 + z_4\,\mathbf{a}_2 - \left(y_4-\frac{1}{2}\right)\mathbf{a}_3$	=	$-b\left(y_4-\frac{1}{2}\right)\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8h)	Hg II
$\mathbf{B_{11}}$	=	$\left(y_4-z_4+\frac{1}{2}\right)\mathbf{a}_1 - z_4\,\mathbf{a}_2 + \left(y_4+\frac{1}{2}\right)\mathbf{a}_3$	=	$b\left(y_4+\frac{1}{2}\right)\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8h)	Hg II
$\mathbf{B_{12}}$	=	$-(y_4+z_4)\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8h)	Hg II
$\mathbf{B_{13}}$	=	$\left(z_5+\frac{1}{4}\right)\mathbf{a}_1 + (x_5+z_5)\,\mathbf{a}_2 + \left(x_5+\frac{1}{4}\right)\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8i)	Hg III
$\mathbf{B_{14}}$	=	$\left(z_5+\frac{1}{4}\right)\mathbf{a}_1 - (x_5-z_5)\,\mathbf{a}_2 - \left(x_5-\frac{1}{4}\right)\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8i)	Hg III
$\mathbf{B_{15}}$	=	$-\left(z_5-\frac{3}{4}\right)\mathbf{a}_1 - (x_5+z_5)\,\mathbf{a}_2 - \left(x_5-\frac{3}{4}\right)\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8i)	Hg III
$\mathbf{B_{16}}$	=	$-\left(z_5-\frac{3}{4}\right)\mathbf{a}_1 + (x_5-z_5)\,\mathbf{a}_2 + \left(x_5+\frac{3}{4}\right)\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8i)	Hg III
$\mathbf{B_{17}}$	=	$\left(z_6+\frac{1}{4}\right)\mathbf{a}_1 + (x_6+z_6)\,\mathbf{a}_2 + \left(x_6+\frac{1}{4}\right)\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8i)	I III
$\mathbf{B_{18}}$	=	$\left(z_6+\frac{1}{4}\right)\mathbf{a}_1 - (x_6-z_6)\,\mathbf{a}_2 - \left(x_6-\frac{1}{4}\right)\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8i)	I III
$\mathbf{B_{19}}$	=	$-\left(z_6-\frac{3}{4}\right)\mathbf{a}_1 - (x_6+z_6)\,\mathbf{a}_2 - \left(x_6-\frac{3}{4}\right)\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8i)	I III
$\mathbf{B_{20}}$	=	$-\left(z_6-\frac{3}{4}\right)\mathbf{a}_1 + (x_6-z_6)\,\mathbf{a}_2 + \left(x_6+\frac{3}{4}\right)\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8i)	I III
$\mathbf{B_{21}}$	=	$(y_7+z_7)\,\mathbf{a}_1 + (x_7+z_7)\,\mathbf{a}_2 + (x_7+y_7)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(16j)	S I

$$\mathbf{B_{22}} = \left(-y_7 + z_7 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - \left(x_7 + y_7 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} - b\left(y_7 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{S I}$$

$$\mathbf{B_{23}} = \left(y_7 - z_7 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - (x_7 + z_7)\,\mathbf{a}_2 + \left(-x_7 + y_7 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} + b\left(y_7 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{S I}$$

$$\mathbf{B_{24}} = -(y_7 + z_7)\,\mathbf{a}_1 + (x_7 - z_7)\,\mathbf{a}_2 + (x_7 - y_7)\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{S I}$$

$$\mathbf{B_{25}} = -(y_7 + z_7)\,\mathbf{a}_1 - (x_7 + z_7)\,\mathbf{a}_2 - (x_7 + y_7)\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{S I}$$

$$\mathbf{B_{26}} = \left(y_7 - z_7 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + (x_7 - z_7)\,\mathbf{a}_2 + \left(x_7 + y_7 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} + b\left(y_7 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{S I}$$

$$\mathbf{B_{27}} = \left(-y_7 + z_7 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + \left(x_7 - y_7 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} - b\left(y_7 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{S I}$$

$$\mathbf{B_{28}} = (y_7 + z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - (x_7 - y_7)\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{S I}$$

References

[1] J. Beck and S. Hedderich, *Synthesis and Crystal Structure of $Hg_3S_2I_2$ and $Hg_3Se_2I_2$, New Members of the $Hg_3E_2X_2$ Family*, Journal of Solid State Chemistry **151**, 73–76 (2000), doi:10.1006/jssc.1999.8624.

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.