

Tl₄HgI₆ Structure: AB6C4_tP22_104_a_2ac_c-001

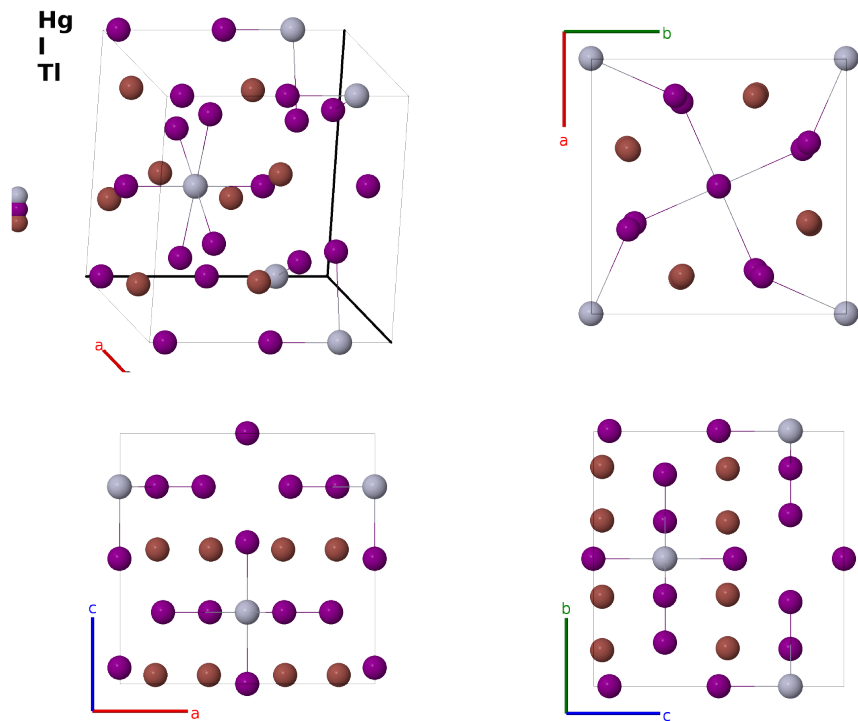
This structure previously used the label(s) **AB6C4_tP22_104_a_2ac_c**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/Z85J>

https://aflow.org/prototype-encyclopedia/AB6C4_tP22_104_a_2ac_c-001

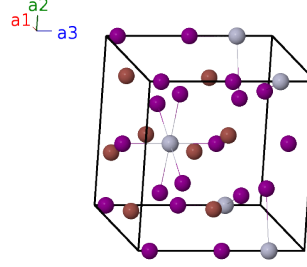


Prototype	HgI ₆ Tl ₄
AFLOW prototype label	AB6C4_tP22_104_a_2ac_c-001
ICSD	250133
CCDC	1716184
Pearson symbol	tP22
Space group number	104
Space group symbol	<i>P4nc</i>
AFLOW prototype command	<code>aflow --proto=AB6C4_tP22_104_a_2ac_c-001</code> <code>--params=a, c/a, z₁, z₂, z₃, x₄, y₄, z₄, x₅, y₅, z₅</code>

- The I-II (2a) site is only occupied 92% of the time.

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	Hg I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c (z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Hg I
$\mathbf{B}_3$	$= z_2 \mathbf{a}_3$	$=$	$c z_2 \hat{\mathbf{z}}$	(2a)	I I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	I I
$\mathbf{B}_5$	$= z_3 \mathbf{a}_3$	$=$	$c z_3 \hat{\mathbf{z}}$	(2a)	I II
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	I II
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + a y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(8c)	I III
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - a y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(8c)	I III
$\mathbf{B}_9$	$= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a y_4 \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(8c)	I III
$\mathbf{B}_{10}$	$= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a y_4 \hat{\mathbf{x}} - a x_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(8c)	I III
$\mathbf{B}_{11}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	I III
$\mathbf{B}_{12}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_4 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	I III
$\mathbf{B}_{13}$	$= -(y_4 - \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (y_4 - \frac{1}{2}) \hat{\mathbf{x}} - a (x_4 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	I III
$\mathbf{B}_{14}$	$= (y_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (y_4 + \frac{1}{2}) \hat{\mathbf{x}} + a (x_4 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	I III
$\mathbf{B}_{15}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} + a y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(8c)	Tl I
$\mathbf{B}_{16}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} - a y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(8c)	Tl I
$\mathbf{B}_{17}$	$= -y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a y_5 \hat{\mathbf{x}} + a x_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(8c)	Tl I
$\mathbf{B}_{18}$	$= y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a y_5 \hat{\mathbf{x}} - a x_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(8c)	Tl I
$\mathbf{B}_{19}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_5 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Tl I
$\mathbf{B}_{20}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_5 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_5 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Tl I
$\mathbf{B}_{21}$	$= -(y_5 - \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (y_5 - \frac{1}{2}) \hat{\mathbf{x}} - a (x_5 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Tl I

$$\mathbf{B}_{22} = \begin{pmatrix} y_5 + \frac{1}{2} \\ x_5 + \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_5 + \frac{1}{2} \\ z_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} z_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 = a \left(y_5 + \frac{1}{2} \right) \hat{\mathbf{x}} + a \left(x_5 + \frac{1}{2} \right) \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2} \right) \hat{\mathbf{z}} \quad (8c) \quad \text{T1 I}$$

References

- [1] D. V. Badikov, V. V. Badikov, G. M. Kuzd'micheva, V. L. Panyutin, V. B. Rybakov, V. I. Chizhikov, G. S. Shevyrdyaeva, and E. S. Shcherbakova, *Growth and X-ray Diffraction Study of Tl_4HgI_6 Crystals*, Inorg. Mater. **40**, 314–320 (2004), doi:10.1023/B:INMA.00000020535.59699.ff.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

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