Sb_2Tl_7 ($L2_2$) Structure: A2B7_cI54_229_e_afh-001

This structure previously used the label(s) `A2B7_cI54_229_e_afh`. Calls to these addresses will be redirected here.

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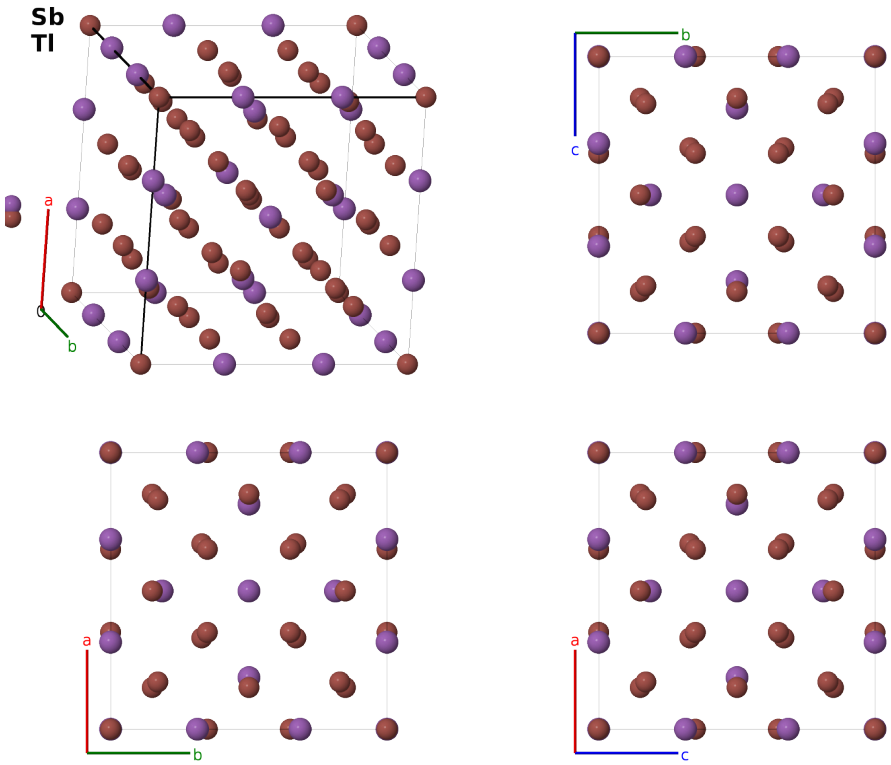
https://aflow.org/prototype-encyclopedia/KM4R

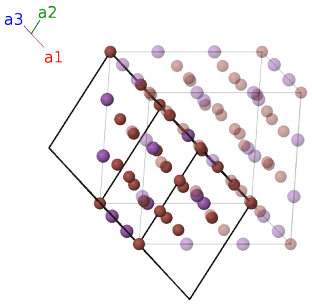
https://aflow.org/prototype-encyclopedia/A2B7_cI54_229_e_afh-001



Prototype	Sb_2Tl_7
AFLOW prototype label	A2B7_cI54_229_e_afh-001
***Strukturbericht* designation**	$L2_2$
ICSD	41816
CCDC	1611567
Pearson symbol	cI54
Space group number	229
Space group symbol	$Im\bar{3}m$
AFLOW prototype command	`aflow --proto=A2B7_cI54_229_e_afh-001 --params=`a, x_2, x_3, y_4

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Tl I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}$	(12e)	Sb I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}$	(12e)	Sb I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{y}}$	(12e)	Sb I
$\mathbf{B_5}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{y}}$	(12e)	Sb I
$\mathbf{B_6}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{z}}$	(12e)	Sb I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{z}}$	(12e)	Sb I
$\mathbf{B_8}$	=	$2x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2 + 2x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16f)	Tl II
$\mathbf{B_9}$	=	$-2x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16f)	Tl II
$\mathbf{B_{10}}$	=	$-2x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(16f)	Tl II
$\mathbf{B_{11}}$	=	$-2x_3\,\mathbf{a}_1$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(16f)	Tl II
$\mathbf{B_{12}}$	=	$2x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(16f)	Tl II
$\mathbf{B_{13}}$	=	$-2x_3\,\mathbf{a}_1 - 2x_3\,\mathbf{a}_2 - 2x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(16f)	Tl II
$\mathbf{B_{14}}$	=	$2x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16f)	Tl II
$\mathbf{B_{15}}$	=	$2x_3\,\mathbf{a}_1$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16f)	Tl II
$\mathbf{B_{16}}$	=	$2y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{y}} + ay_4\,\hat{\mathbf{z}}$	(24h)	Tl III
$\mathbf{B_{17}}$	=	$y_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{y}} + ay_4\,\hat{\mathbf{z}}$	(24h)	Tl III
$\mathbf{B_{18}}$	=	$-y_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{y}} - ay_4\,\hat{\mathbf{z}}$	(24h)	Tl III
$\mathbf{B_{19}}$	=	$-2y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{y}} - ay_4\,\hat{\mathbf{z}}$	(24h)	Tl III
$\mathbf{B_{20}}$	=	$y_4\,\mathbf{a}_1 + 2y_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{z}}$	(24h)	Tl III
$\mathbf{B_{21}}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{z}}$	(24h)	Tl III
$\mathbf{B_{22}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{z}}$	(24h)	Tl III
$\mathbf{B_{23}}$	=	$-y_4\,\mathbf{a}_1 - 2y_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{z}}$	(24h)	Tl III
$\mathbf{B_{24}}$	=	$y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + 2y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}}$	(24h)	Tl III
$\mathbf{B_{25}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2$	=	$-ay_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}}$	(24h)	Tl III
$\mathbf{B_{26}}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2$	=	$ay_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}}$	(24h)	Tl III
$\mathbf{B_{27}}$	=	$-y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - 2y_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}}$	(24h)	Tl III

References

[1] R. Stokhuyzen, C. Chieh, and W. B. Pearson, *Crystal Structure of Sb_2Tl_7*, Can. J. Chem. **55**, 1120–1122 (1977), doi:10.1139/v77-157.

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.

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