

Intermediate Temperature Tetragonal TlS Structure: AB_tP64_92_2a3b_4b-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/X71C>

https://aflow.org/prototype-encyclopedia/AB_tP64_92_2a3b_4b-001

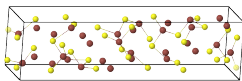
Prototype	STl
AFLOW prototype label	AB_tP64_92_2a3b_4b-001
ICSD	78162
CCDC	1638489
Pearson symbol	tP64
Space group number	92
Space group symbol	$P4_12_12$
AFLOW prototype command	<pre>aflow --proto=AB_tP64_92_2a3b_4b-001 --params=a, c/a, x₁, x₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈, x₉, y₉, z₉</pre>

- TlS occurs naturally in three forms (Villars, 2018):
 - The ground state is tetragonal in the TlSe (*B37*) structure which (Villars, 2018) calls “Tet-I” and (Kishida, 1994) calls “Type I.”
 - An intermediate tetragonal structure, which (Villars, 2018) calls “Tetragonal II,” and (Kashida, 1994) calls Type III. (this structure)
 - A high temperature monoclinic structure, called “Mon” by (Villars, 2018) and “Type II” by (Kishida, 1994).

Simple Tetragonal primitive vectors

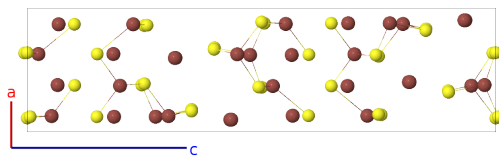
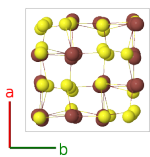
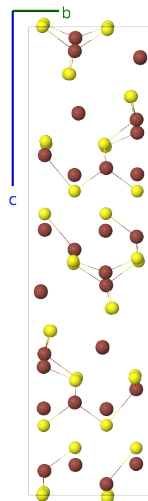
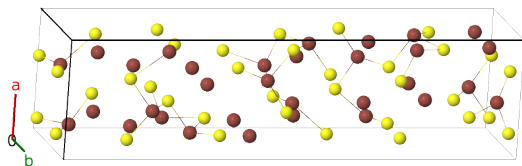
$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$

$\mathbf{a}_1$
 $\mathbf{a}_2$
 $\mathbf{a}_3$



Basis vectors

S
Ti



$\mathbf{B}_{30} =$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{3}{4}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	S V
$\mathbf{B}_{31} =$	$y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8b)	S V
$\mathbf{B}_{32} =$	$-y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	S V
$\mathbf{B}_{33} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8b)	Tl I
$\mathbf{B}_{34} =$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Tl I
$\mathbf{B}_{35} =$	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Tl I
$\mathbf{B}_{36} =$	$(y_6 + \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{3}{4}) \mathbf{a}_3$	$=$	$a(y_6 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	Tl I
$\mathbf{B}_{37} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{4}) \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Tl I
$\mathbf{B}_{38} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{3}{4}) \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	Tl I
$\mathbf{B}_{39} =$	$y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8b)	Tl I
$\mathbf{B}_{40} =$	$-y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Tl I
$\mathbf{B}_{41} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8b)	Tl II
$\mathbf{B}_{42} =$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Tl II
$\mathbf{B}_{43} =$	$-(y_7 - \frac{1}{2}) \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-a(y_7 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Tl II
$\mathbf{B}_{44} =$	$(y_7 + \frac{1}{2}) \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{3}{4}) \mathbf{a}_3$	$=$	$a(y_7 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	Tl II
$\mathbf{B}_{45} =$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - (z_7 - \frac{1}{4}) \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_7 - \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Tl II
$\mathbf{B}_{46} =$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - (z_7 - \frac{3}{4}) \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_7 - \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	Tl II
$\mathbf{B}_{47} =$	$y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8b)	Tl II
$\mathbf{B}_{48} =$	$-y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Tl II
$\mathbf{B}_{49} =$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8b)	Tl III
$\mathbf{B}_{50} =$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Tl III
$\mathbf{B}_{51} =$	$-(y_8 - \frac{1}{2}) \mathbf{a}_1 + (x_8 + \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-a(y_8 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_8 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Tl III
$\mathbf{B}_{52} =$	$(y_8 + \frac{1}{2}) \mathbf{a}_1 - (x_8 - \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{3}{4}) \mathbf{a}_3$	$=$	$a(y_8 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_8 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	Tl III
$\mathbf{B}_{53} =$	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{4}) \mathbf{a}_3$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Tl III
$\mathbf{B}_{54} =$	$(x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{3}{4}) \mathbf{a}_3$	$=$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_8 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	Tl III
$\mathbf{B}_{55} =$	$y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$ay_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8b)	Tl III
$\mathbf{B}_{56} =$	$-y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Tl III
$\mathbf{B}_{57} =$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8b)	Tl IV
$\mathbf{B}_{58} =$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - ay_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Tl IV
$\mathbf{B}_{59} =$	$-(y_9 - \frac{1}{2}) \mathbf{a}_1 + (x_9 + \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-a(y_9 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_9 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Tl IV

$$\begin{aligned}
\mathbf{B}_{60} &= \begin{pmatrix} (y_9 + \frac{1}{2}) \mathbf{a}_1 - (x_9 - \frac{1}{2}) \mathbf{a}_2 + \\ (z_9 + \frac{3}{4}) \mathbf{a}_3 \end{pmatrix} = a \left(y_9 + \frac{1}{2} \right) \hat{\mathbf{x}} - a \left(x_9 - \frac{1}{2} \right) \hat{\mathbf{y}} + c \left(z_9 + \frac{3}{4} \right) \hat{\mathbf{z}} & (8b) & \text{Tl IV} \\
\mathbf{B}_{61} &= \begin{pmatrix} - (x_9 - \frac{1}{2}) \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - \\ (z_9 - \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_9 - \frac{1}{2} \right) \hat{\mathbf{x}} + a \left(y_9 + \frac{1}{2} \right) \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{4} \right) \hat{\mathbf{z}} & (8b) & \text{Tl IV} \\
\mathbf{B}_{62} &= \begin{pmatrix} (x_9 + \frac{1}{2}) \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 - \\ (z_9 - \frac{3}{4}) \mathbf{a}_3 \end{pmatrix} = a \left(x_9 + \frac{1}{2} \right) \hat{\mathbf{x}} - a \left(y_9 - \frac{1}{2} \right) \hat{\mathbf{y}} - c \left(z_9 - \frac{3}{4} \right) \hat{\mathbf{z}} & (8b) & \text{Tl IV} \\
\mathbf{B}_{63} &= y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 = ay_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (8b) & \text{Tl IV} \\
\mathbf{B}_{64} &= -y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - \left(z_9 - \frac{1}{2} \right) \mathbf{a}_3 = -ay_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{2} \right) \hat{\mathbf{z}} & (8b) & \text{Tl IV}
\end{aligned}$$

References

- [1] S. Kashida and K. Nakamura, *An X-Ray Study of the Polymorphism in Thallium Monosulfide: The Structure of Two Tetragonal Forms*, J. Solid State Chem. **110**, 264–269 (1994), doi:10.1006/jssc.1994.1168.

Found in

- [1] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Sulfur-Thallium Binary Phase Diagram (1990 Okamoto H.). Copyright ©2006-2018 ASM International.

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