Intermediate Temperature Tetragonal TlS Structure: AB_tP64_92_2a3b_4b-001

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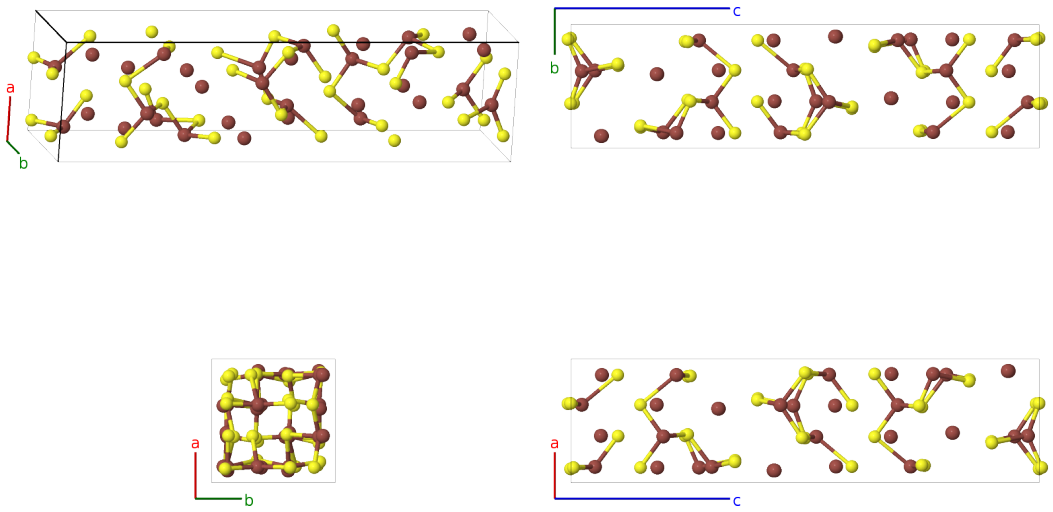
https://aflow.org/p/X71C

https://aflow.org/p/AB_tP64_92_2a3b_4b-001

S
Tl

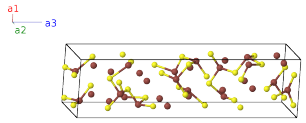


Prototype	STl
AFLOW prototype label	AB_tP64_92_2a3b_4b-001
ICSD	78162
Pearson symbol	tP64
Space group number	92
Space group symbol	$P4_12_12$
AFLOW prototype command	`aflow --proto=AB_tP64_92_2a3b_4b-001 --params=`$a, c/a, x_1, x_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$

- 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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}}$	(4a)	S I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	S I
$\mathbf{B_3}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	S I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	S I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(4a)	S II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	S II
$\mathbf{B_7}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	S II
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	S II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8b)	S III
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	S III
$\mathbf{B_{11}}$	=	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	S III
$\mathbf{B_{12}}$	=	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8b)	S III
$\mathbf{B_{13}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	S III
$\mathbf{B_{14}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8b)	S III
$\mathbf{B_{15}}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8b)	S III
$\mathbf{B_{16}}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	S III
$\mathbf{B_{17}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8b)	S IV
$\mathbf{B_{18}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	S IV
$\mathbf{B_{19}}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	S IV
$\mathbf{B_{20}}$	=	$\left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8b)	S IV
$\mathbf{B_{21}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	S IV
$\mathbf{B_{22}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_4 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8b)	S IV
$\mathbf{B_{23}}$	=	$y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8b)	S IV
$\mathbf{B_{24}}$	=	$-y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	S IV
$\mathbf{B_{25}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8b)	S V

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\begin{array}{lcccccc}
\mathbf{B_{26}} & = & -x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{S V} \\
\mathbf{B_{27}} & = & -\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_5+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5+\frac{1}{4}\right)\,\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}{4}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{S V} \\
\mathbf{B_{28}} & = & \left(y_5+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5+\frac{3}{4}\right)\,\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{3}{4}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{S V} \\
\mathbf{B_{29}} & = & -\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_5-\frac{1}{4}\right)\,\mathbf{a}_3 & = & -a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_5-\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{S V} \\
\mathbf{B_{30}} & = & \left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_5-\frac{3}{4}\right)\,\mathbf{a}_3 & = & a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_5-\frac{3}{4}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{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}} & \text{(8b)} & \text{S V} \\
\mathbf{B_{32}} & = & -y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - \left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - c\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{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}} & \text{(8b)} & \text{Tl I} \\
\mathbf{B_{34}} & = & -x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{Tl I} \\
\mathbf{B_{35}} & = & -\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_6+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6+\frac{1}{4}\right)\,\mathbf{a}_3 & = & -a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{Tl I} \\
\mathbf{B_{36}} & = & \left(y_6+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_6-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6+\frac{3}{4}\right)\,\mathbf{a}_3 & = & a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_6+\frac{3}{4}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{Tl I} \\
\mathbf{B_{37}} & = & -\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_6-\frac{1}{4}\right)\,\mathbf{a}_3 & = & -a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_6-\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{Tl I} \\
\mathbf{B_{38}} & = & \left(x_6+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6-\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_6-\frac{3}{4}\right)\,\mathbf{a}_3 & = & a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_6-\frac{3}{4}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{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}} & \text{(8b)} & \text{Tl I} \\
\mathbf{B_{40}} & = & -y_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - \left(z_6-\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ay_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - c\left(z_6-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{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}} & \text{(8b)} & \text{Tl II} \\
\mathbf{B_{42}} & = & -x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_7\,\hat{\mathbf{x}} - ay_7\,\hat{\mathbf{y}} + c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{Tl II} \\
\mathbf{B_{43}} & = & -\left(y_7-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_7+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_7+\frac{1}{4}\right)\,\mathbf{a}_3 & = & -a\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_7+\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{Tl II} \\
\mathbf{B_{44}} & = & \left(y_7+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_7-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_7+\frac{3}{4}\right)\,\mathbf{a}_3 & = & a\left(y_7+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_7+\frac{3}{4}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{Tl II} \\
\mathbf{B_{45}} & = & -\left(x_7-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_7+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_7-\frac{1}{4}\right)\,\mathbf{a}_3 & = & -a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_7+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_7-\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{Tl II} \\
\mathbf{B_{46}} & = & \left(x_7+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_7-\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_7-\frac{3}{4}\right)\,\mathbf{a}_3 & = & a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_7-\frac{3}{4}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{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}} & \text{(8b)} & \text{Tl II} \\
\mathbf{B_{48}} & = & -y_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - \left(z_7-\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ay_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - c\left(z_7-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{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}} & \text{(8b)} & \text{Tl III} \\
\mathbf{B_{50}} & = & -x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_8\,\hat{\mathbf{x}} - ay_8\,\hat{\mathbf{y}} + c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{Tl III} \\
\mathbf{B_{51}} & = & -\left(y_8-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_8+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_8+\frac{1}{4}\right)\,\mathbf{a}_3 & = & -a\left(y_8-\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_8+\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_8+\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{Tl III} \\
\mathbf{B_{52}} & = & \left(y_8+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_8-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_8+\frac{3}{4}\right)\,\mathbf{a}_3 & = & a\left(y_8+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_8-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_8+\frac{3}{4}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{Tl III} \\
\mathbf{B_{53}} & = & -\left(x_8-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_8+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_8-\frac{1}{4}\right)\,\mathbf{a}_3 & = & -a\left(x_8-\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_8+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_8-\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{Tl III} \\
\mathbf{B_{54}} & = & \left(x_8+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_8-\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_8-\frac{3}{4}\right)\,\mathbf{a}_3 & = & a\left(x_8+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_8-\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_8-\frac{3}{4}\right)\,\hat{\mathbf{z}} & \text{(8b)} & \text{Tl III}
\end{array}
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$\mathbf{B_{55}}$	=	$y_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$ay_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(8b)	Tl III
$\mathbf{B_{56}}$	=	$-y_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{58}}$	=	$-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} - ay_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	Tl IV
$\mathbf{B_{59}}$	=	$-\left(y_9 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_9 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_9 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(y_9 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_9 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	Tl IV
$\mathbf{B_{60}}$	=	$\left(y_9 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_9 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_9 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(y_9 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_9 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_9 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8b)	Tl IV
$\mathbf{B_{61}}$	=	$-\left(x_9 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_9 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_9 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_9 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_9 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	Tl IV
$\mathbf{B_{62}}$	=	$\left(x_9 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_9 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_9 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_9 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_9 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8b)	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)	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)	Tl IV

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