Tl_4S_3 Structure: A3B4_mP28_14_3e_4e-001

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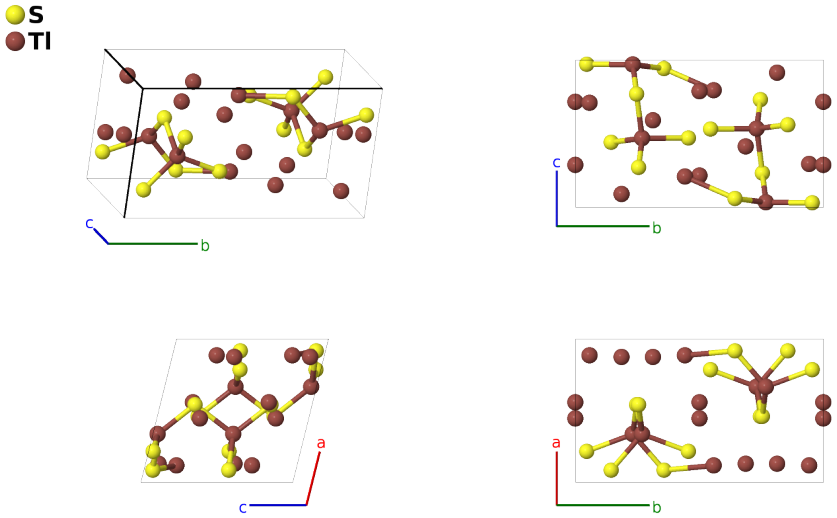
https://aflow.org/p/A3B4_mP28_14_3e_4e-001

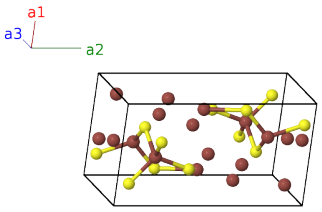


Prototype	S_3Tl_4
AFLOW prototype label	A3B4_mP28_14_3e_4e-001
ICSD	2647
Pearson symbol	mP28
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	`aflow --proto=A3B4_mP28_14_3e_4e-001 --params=`$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

- (Leclerc, 1973) give the structural information in the $P2_1/a$ (unique axis c) setting of space group #14. We used FINDSYM to transform this to the $P2_1/c$ (unique axis b) setting.

Simple Monoclinic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 + \left(y_1+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_1-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_1 + c\left(z_1-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_1-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-\left(ax_1 + cz_1\cos\beta\right)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B_4}$	=	$x_1\,\mathbf{a}_1 - \left(y_1-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_1 + c\left(z_1+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_2 + c\left(z_2-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-\left(ax_2 + cz_2\cos\beta\right)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B_8}$	=	$x_2\,\mathbf{a}_1 - \left(y_2-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_2 + c\left(z_2+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	S III
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_3 + c\left(z_3-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	S III
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-\left(ax_3 + cz_3\cos\beta\right)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	S III
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a}_1 - \left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_3 + c\left(z_3+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	S III
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	Tl I
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_4 + c\left(z_4-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_4-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Tl I
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-\left(ax_4 + cz_4\cos\beta\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	Tl I
$\mathbf{B_{16}}$	=	$x_4\,\mathbf{a}_1 - \left(y_4-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_4 + c\left(z_4+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Tl I
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	Tl II
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 + \left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_5 + c\left(z_5-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_5-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Tl II
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\left(ax_5 + cz_5\cos\beta\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	Tl II
$\mathbf{B_{20}}$	=	$x_5\,\mathbf{a}_1 - \left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_5 + c\left(z_5+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Tl II
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	Tl III
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1 + \left(y_6+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_6-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_6 + c\left(z_6-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_6-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Tl III
$\mathbf{B_{23}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\left(ax_6 + cz_6\cos\beta\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	Tl III
$\mathbf{B_{24}}$	=	$x_6\,\mathbf{a}_1 - \left(y_6-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_6 + c\left(z_6+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Tl III
$\mathbf{B_{25}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4e)	Tl IV
$\mathbf{B_{26}}$	=	$-x_7\,\mathbf{a}_1 + \left(y_7+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_7-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_7 + c\left(z_7-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_7+\frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_7-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Tl IV
$\mathbf{B_{27}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-\left(ax_7 + cz_7\cos\beta\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(4e)	Tl IV

$\mathbf{B_{28}}$	$= x_7\,\mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\left(ax_7 + c\left(z_7 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} -$ $b\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Tl IV

References

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