

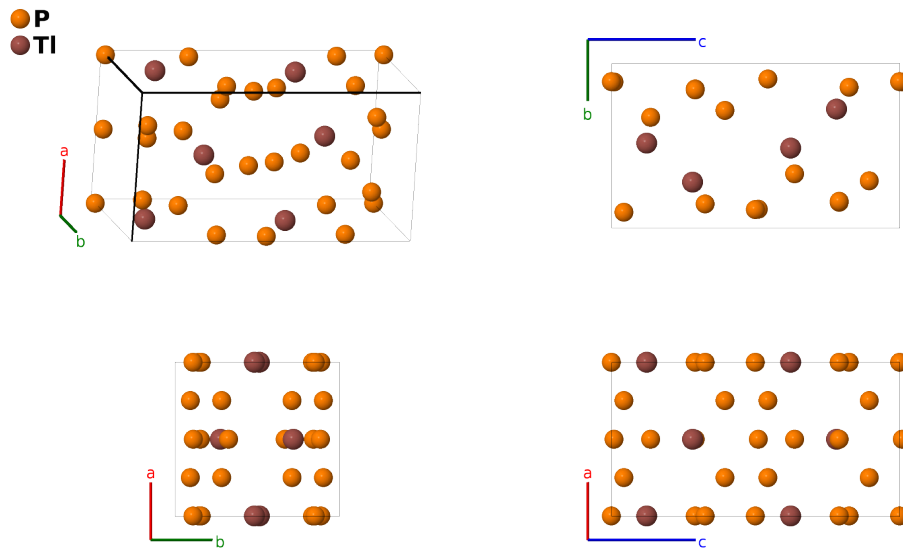
TlP₅ Structure: A5B_oP24_26_3a3b2c_ab-001

This structure originally had the label **A5B_oP24_26_3a3b2c_ab**. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

<https://aflow.org/p/AHE7>

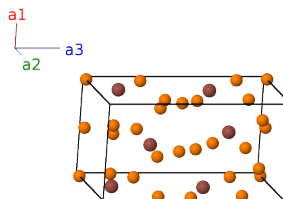
https://aflow.org/p/A5B_oP24_26_3a3b2c_ab-001



Prototype	P ₅ Tl
AFLOW prototype label	A5B_oP24_26_3a3b2c_ab-001
ICSD	15021
Pearson symbol	oP24
Space group number	26
Space group symbol	<i>Pmc</i> 2 ₁
AFLOW prototype command	aflow --proto=A5B_oP24_26_3a3b2c_ab-001 --params=a, b/a, c/a, y ₁ , z ₁ , y ₂ , z ₂ , y ₃ , z ₃ , y ₄ , z ₄ , y ₅ , z ₅ , y ₆ , z ₆ , y ₇ , z ₇ , y ₈ , z ₈ , x ₉ , y ₉ , z ₉ , x ₁₀ , y ₁₀ , z ₁₀

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2a)	P I
\mathbf{B}_2	$= -y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	P I
\mathbf{B}_3	$= y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2a)	P II
\mathbf{B}_4	$= -y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	P II
\mathbf{B}_5	$= y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2a)	P III
\mathbf{B}_6	$= -y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	P III
\mathbf{B}_7	$= y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2a)	Tl I
\mathbf{B}_8	$= -y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Tl I
\mathbf{B}_9	$= \frac{1}{2} \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(2b)	P IV
\mathbf{B}_{10}	$= \frac{1}{2} \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	P IV
\mathbf{B}_{11}	$= \frac{1}{2} \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(2b)	P V
\mathbf{B}_{12}	$= \frac{1}{2} \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	P V
\mathbf{B}_{13}	$= \frac{1}{2} \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(2b)	P VI
\mathbf{B}_{14}	$= \frac{1}{2} \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	P VI
\mathbf{B}_{15}	$= \frac{1}{2} \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(2b)	Tl II
\mathbf{B}_{16}	$= \frac{1}{2} \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Tl II
\mathbf{B}_{17}	$= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(4c)	P VII
\mathbf{B}_{18}	$= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	P VII
\mathbf{B}_{19}	$= x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	P VII
\mathbf{B}_{20}	$= -x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(4c)	P VII
\mathbf{B}_{21}	$= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(4c)	P VIII
\mathbf{B}_{22}	$= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	P VIII
\mathbf{B}_{23}	$= x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	P VIII
\mathbf{B}_{24}	$= -x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(4c)	P VIII

References

- [1] O. Olofsson and J. Gullman, *The Crystal Structure of TlP₅*, Acta Chem. Scand. **25**, 1327–1337 (1971), doi:10.3891/acta.chem.scand.25-132.

Found in

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