

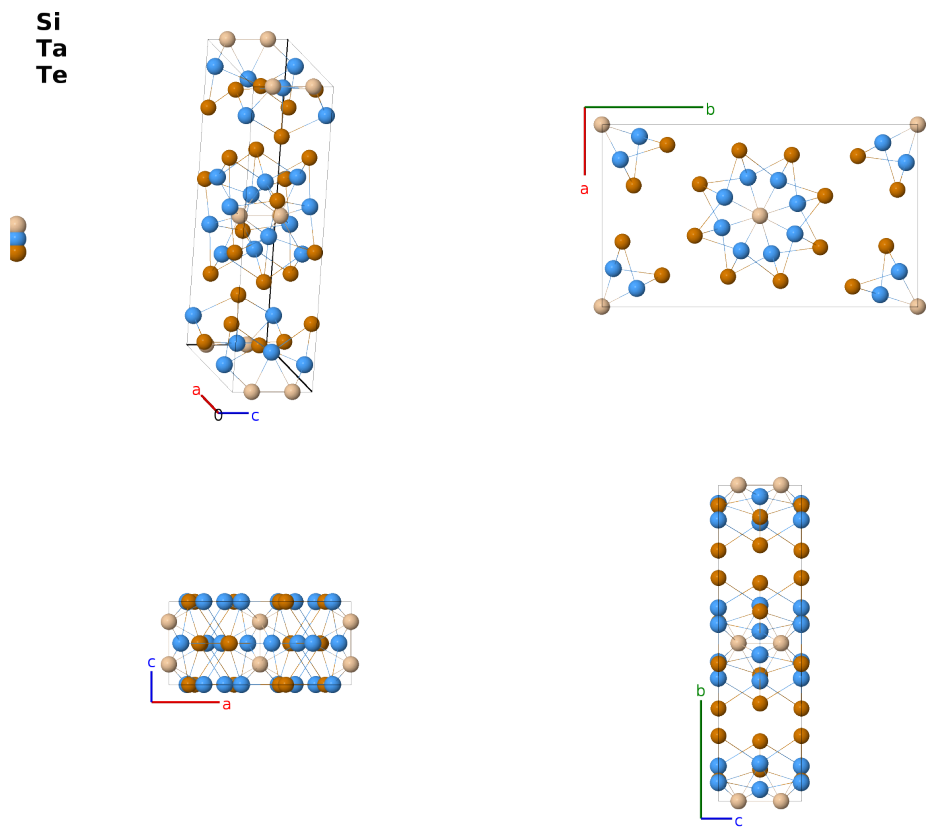
Ta₄SiTe₄ Structure: AB4C4_oP36_55_e_2g2h_2g2h-001

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<https://aflow.org/prototype-encyclopedia/UXGR>

https://aflow.org/prototype-encyclopedia/AB4C4_oP36_55_e_2g2h_2g2h-001



Prototype	SiTa ₄ Te ₄
AFLOW prototype label	AB4C4_oP36_55_e_2g2h_2g2h-001
ICSD	40207
CCDC	1610112
Pearson symbol	oP36
Space group number	55
Space group symbol	<i>Pbam</i>
AFLOW prototype command	<code>aflow --proto=AB4C4_oP36_55_e_2g2h_2g2h-001</code> <code>--params=a, b/a, c/a, z₁, x₂, y₂, x₃, y₃, x₄, y₄, x₅, y₅, x₆, y₆, x₇, y₇, x₈, y₈, x₉, y₉</code>

Other compounds with this structure

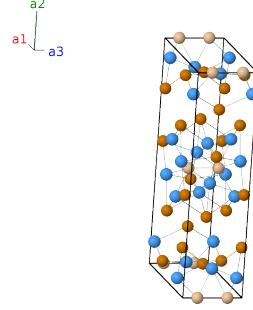
Nb₄SiTe₄, Ta₄CoTe₄

Simple Orthorhombic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B}_3$	$= -z_1 \mathbf{a}_3$	$=$	$-cz_1 \hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}}$	(4g)	Ta I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}}$	(4g)	Ta I
$\mathbf{B}_7$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Ta I
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Ta I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}}$	(4g)	Ta II
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}}$	(4g)	Ta II
$\mathbf{B}_{11}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Ta II
$\mathbf{B}_{12}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Ta II
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}}$	(4g)	Te I
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}}$	(4g)	Te I
$\mathbf{B}_{15}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Te I
$\mathbf{B}_{16}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Te I
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}}$	(4g)	Te II
$\mathbf{B}_{18}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}}$	(4g)	Te II
$\mathbf{B}_{19}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Te II
$\mathbf{B}_{20}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Te II
$\mathbf{B}_{21}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h)	Ta III
$\mathbf{B}_{22}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h)	Ta III
$\mathbf{B}_{23}$	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h)	Ta III
$\mathbf{B}_{24}$	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h)	Ta III
$\mathbf{B}_{25}$	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h)	Ta IV

$$\begin{aligned}
\mathbf{B}_{26} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Ta IV} \\
\mathbf{B}_{27} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Ta IV} \\
\mathbf{B}_{28} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= a\left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Ta IV} \\
\mathbf{B}_{29} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Te III} \\
\mathbf{B}_{30} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Te III} \\
\mathbf{B}_{31} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Te III} \\
\mathbf{B}_{32} &= \left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_8 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Te III} \\
\mathbf{B}_{33} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Te IV} \\
\mathbf{B}_{34} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Te IV} \\
\mathbf{B}_{35} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Te IV} \\
\mathbf{B}_{36} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Te IV}
\end{aligned}$$

References

- [1] M. E. Badding and F. J. DiSalvo, *Synthesis and structure of tantalum silicide telluride, Ta₄SiTe₄, a new low-dimensional material*, Inorg. Chem. **29**, 3952–3954 (1990), doi:10.1021/ic00345a009.

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