Ta$_4$SiTe$_4$ Structure:
AB4C4_oP36_55_e_2g2h_2g2h-001

https://aflow.org/p/UXGR

https://aflow.org/p/AB4C4_oP36_55_e_2g2h_2g2h-001
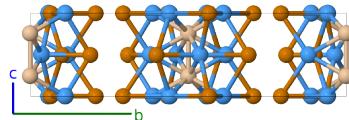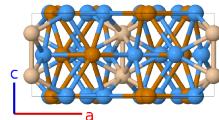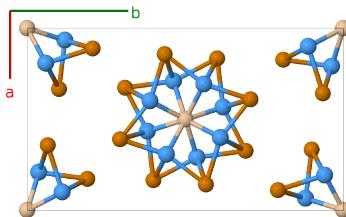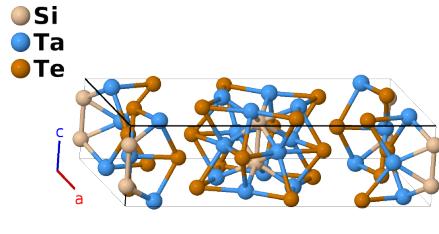
Prototype	SiTa$_4$Te$_4$
AFLOW prototype label	AB4C4_oP36_55_e_2g2h_2g2h-001
ICSD	40207
Pearson symbol	oP36
Space group number	55
Space group symbol	*Pbam*
AFLOW prototype command	aflow --proto=AB4C4_oP36_55_e_2g2h_2g2h-001 --params=$a, b/a, c/a, z_1, x_2, y_2, x_3, y_3, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7, x_8, y_8, x_9, y_9$

Other compounds with this structure
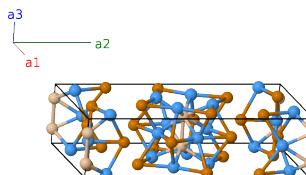
Nb$_4$SiTe$_4$, Ta$_4$CoTe$_4$

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
$\mathbf{B_7}$	$=$	$-\left(x_2 - \frac{1}{2}\right)\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\mathbf{a}_2$	$=$	$-a\left(x_2 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}}$	(4g)	Ta I
$\mathbf{B_8}$	$=$	$\left(x_2 + \frac{1}{2}\right)\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\mathbf{a}_2$	$=$	$a\left(x_2 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\hat{\mathbf{y}}$	(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
$\mathbf{B_{11}}$	$=$	$-\left(x_3 - \frac{1}{2}\right)\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\mathbf{a}_2$	$=$	$-a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}}$	(4g)	Ta II
$\mathbf{B_{12}}$	$=$	$\left(x_3 + \frac{1}{2}\right)\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\mathbf{a}_2$	$=$	$a\left(x_3 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}}$	(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
$\mathbf{B_{15}}$	$=$	$-\left(x_4 - \frac{1}{2}\right)\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\mathbf{a}_2$	$=$	$-a\left(x_4 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}}$	(4g)	Te I
$\mathbf{B_{16}}$	$=$	$\left(x_4 + \frac{1}{2}\right)\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\mathbf{a}_2$	$=$	$a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}}$	(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
$\mathbf{B_{19}}$	$=$	$-\left(x_5 - \frac{1}{2}\right)\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\mathbf{a}_2$	$=$	$-a\left(x_5 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}}$	(4g)	Te II
$\mathbf{B_{20}}$	$=$	$\left(x_5 + \frac{1}{2}\right)\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\mathbf{a}_2$	$=$	$a\left(x_5 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}}$	(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
$\mathbf{B_{23}}$	$=$	$-\left(x_6 - \frac{1}{2}\right)\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	$=$	$-a\left(x_6 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Ta III
$\mathbf{B_{24}}$	$=$	$\left(x_6 + \frac{1}{2}\right)\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	$=$	$a\left(x_6 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{26}}$	$=$	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	$=$	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	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)	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)	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)	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)	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)	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)	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)	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)	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)	Te IV

$$\mathbf{B_{36}} \quad = \quad \left(x_9 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_9 - \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 \quad = \quad a\left(x_9 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_9 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \qquad (4h) \qquad \text{Te IV}$$

References

[1] M. E. Badding and F. J. DiSalvo, *Synthesis and structure of tantalum silicide telluride, Ta_4SiTe_4, a new low-dimensional material*, Inorg. Chem. **29**, 3952–3954 (1990), doi:10.1021/ic00345a009.