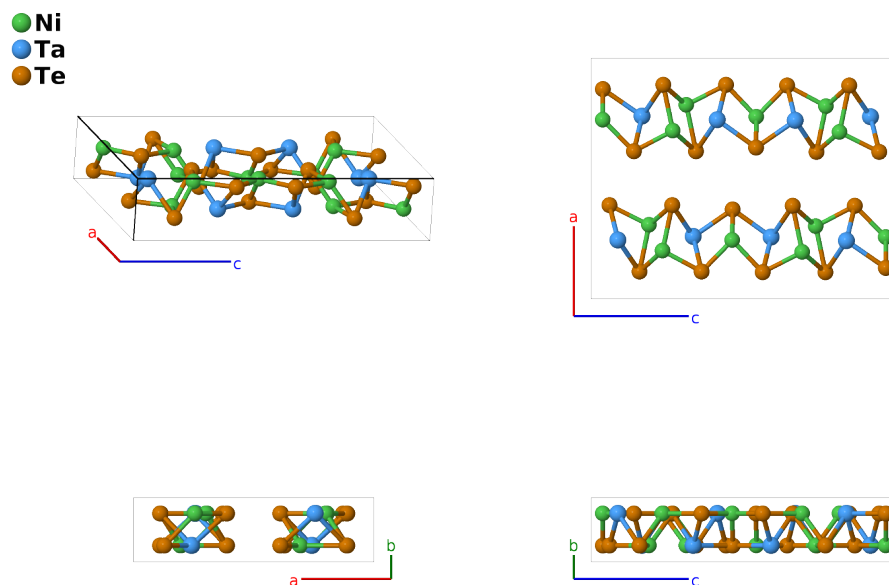


# Ta<sub>2</sub>Ni<sub>3</sub>Te<sub>5</sub> Structure: A3B2C5\_oP40\_62\_3c\_2c\_5c-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://aflow.org/p/72A0>

[https://aflow.org/p/A3B2C5\\_oP40\\_62\\_3c\\_2c\\_5c-001](https://aflow.org/p/A3B2C5_oP40_62_3c_2c_5c-001)



<b>Prototype</b>	Ni <sub>3</sub> Ta <sub>2</sub> Te <sub>5</sub>
<b>AFLOW prototype label</b>	A3B2C5_oP40_62_3c_2c_5c-001
<b>ICSD</b>	none
<b>Pearson symbol</b>	oP40
<b>Space group number</b>	62
<b>Space group symbol</b>	<i>Pnma</i>
<b>AFLOW prototype command</b>	<code>aflow --proto=A3B2C5_oP40_62_3c_2c_5c-001 --params=a, b/a, c/a, x<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, z<sub>8</sub>, x<sub>9</sub>, z<sub>9</sub>, x<sub>10</sub>, z<sub>10</sub></code>

## Other compounds with this structure

Ta<sub>2</sub>Pd<sub>3</sub>Te<sub>5</sub>

- We wish to thank Petra Lipsky, FIZ Karlsruhe - Leibniz-Institut für Informationsinfrastruktur, who provided us with the data referenced in (Tremel, 1991). For more information about the FIZ Karlsruhe archive, see FIZ Karlsruhe.

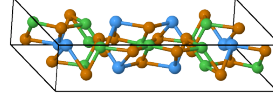
## Simple Orthorhombic primitive vectors



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

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

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



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	Ni I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Ni I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	Ni I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Ni I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	Ni II
$\mathbf{B}_6$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Ni II
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	Ni II
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Ni II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	Ni III
$\mathbf{B}_{10}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Ni III
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	Ni III
$\mathbf{B}_{12}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Ni III
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	Ta I
$\mathbf{B}_{14}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Ta I
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4c)	Ta I
$\mathbf{B}_{16}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Ta I
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	Ta II
$\mathbf{B}_{18}$	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Ta II
$\mathbf{B}_{19}$	$= -x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4c)	Ta II
$\mathbf{B}_{20}$	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Ta II
$\mathbf{B}_{21}$	$= x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	Te I
$\mathbf{B}_{22}$	$= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Te I
$\mathbf{B}_{23}$	$= -x_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4c)	Te I
$\mathbf{B}_{24}$	$= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Te I

$$\begin{aligned}
\mathbf{B}_{25} &= x_7 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_7 \mathbf{a}_3 &= ax_7 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} &(4c) &\text{Te II} \\
\mathbf{B}_{26} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + &= -a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{Te II} \\
&\quad \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{27} &= -x_7 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -ax_7 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(4c) &\text{Te II} \\
\mathbf{B}_{28} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{Te II} \\
\mathbf{B}_{29} &= x_8 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_8 \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} &(4c) &\text{Te III} \\
\mathbf{B}_{30} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + &= -a \left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{Te III} \\
&\quad \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{31} &= -x_8 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_8 \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} &(4c) &\text{Te III} \\
\mathbf{B}_{32} &= \left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{Te III} \\
\mathbf{B}_{33} &= x_9 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_9 \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} &(4c) &\text{Te IV} \\
\mathbf{B}_{34} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + &= -a \left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{Te IV} \\
&\quad \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{35} &= -x_9 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_9 \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} &(4c) &\text{Te IV} \\
\mathbf{B}_{36} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{Te IV} \\
\mathbf{B}_{37} &= x_{10} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= ax_{10} \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} &(4c) &\text{Te V} \\
\mathbf{B}_{38} &= -\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + &= -a \left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c \left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{Te V} \\
&\quad \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{39} &= -x_{10} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= -ax_{10} \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(4c) &\text{Te V} \\
\mathbf{B}_{40} &= \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - &= a \left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c \left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{Te V} \\
&\quad \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3
\end{aligned}$$

## References

- [1] W. Tremel, *Isolated and Condensed Ta<sub>2</sub>Ni<sub>2</sub> Clusters in the Layered Tellurides Ta<sub>2</sub>Ni<sub>2</sub>Te<sub>4</sub> and Ta<sub>2</sub>Ni<sub>3</sub>Te<sub>5</sub>*, *Angew. Chem. Int. Ed.* **30**, 840–843 (1991), doi:10.1002/anie.199108401.