

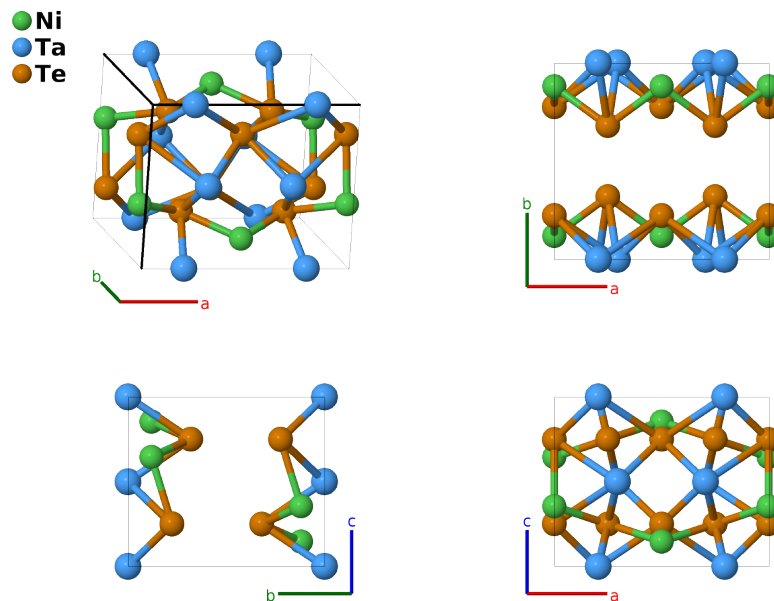
# TaNiTe<sub>2</sub> Structure: ABC2\_oP16\_53\_h\_e\_gh-001

This structure originally had the label `ABC2_oP16_53_h_e_gh`. Calls to that address will be redirected here.

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

[https://aflow.org/p/ABC2\\_oP16\\_53\\_h\\_e\\_gh-001](https://aflow.org/p/ABC2_oP16_53_h_e_gh-001)

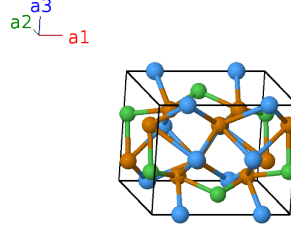


<b>Prototype</b>	NiTaTe <sub>2</sub>
<b>AFLOW prototype label</b>	ABC2_oP16_53_h_e_gh-001
<b>ICSD</b>	71063
<b>Pearson symbol</b>	oP16
<b>Space group number</b>	53
<b>Space group symbol</b>	<i>Pmna</i>
<b>AFLOW prototype command</b>	<code>aflow --proto=ABC2_oP16_53_h_e_gh-001 --params=a,b/a,c/a,x1,y2,y3,z3,y4,z4</code>

- Our original published version of this structure (Hicks, 2019) has incorrect lattice parameters. These are corrected here, and now show the layered structure of TaNiTe<sub>2</sub>.
- The origin of the *y*-axis has been shifted by *b*/2 from that of (Tremel, 1991), moving the tantalum atoms from the (4f) Wyckoff position to (4e).

## 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
$\mathbf{B}_1$	$x_1 \mathbf{a}_1$	=	$a x_1 \hat{\mathbf{x}}$	(4e)	Ta I
$\mathbf{B}_2$	$-(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	=	$-a (x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4e)	Ta I
$\mathbf{B}_3$	$-x_1 \mathbf{a}_1$	=	$-a x_1 \hat{\mathbf{x}}$	(4e)	Ta I
$\mathbf{B}_4$	$(x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	=	$a (x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4e)	Ta I
$\mathbf{B}_5$	$\frac{1}{4} \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4g)	Te I
$\mathbf{B}_6$	$\frac{1}{4} \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{1}{4} a \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4g)	Te I
$\mathbf{B}_7$	$\frac{3}{4} \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{3}{4} a \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4g)	Te I
$\mathbf{B}_8$	$\frac{3}{4} \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{3}{4} a \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4g)	Te I
$\mathbf{B}_9$	$y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4h)	Ni I
$\mathbf{B}_{10}$	$\frac{1}{2} \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	Ni I
$\mathbf{B}_{11}$	$\frac{1}{2} \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	Ni I
$\mathbf{B}_{12}$	$-y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-b y_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(4h)	Ni I
$\mathbf{B}_{13}$	$y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4h)	Te II
$\mathbf{B}_{14}$	$\frac{1}{2} \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	Te II
$\mathbf{B}_{15}$	$\frac{1}{2} \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} - c (z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	Te II
$\mathbf{B}_{16}$	$-y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-b y_4 \hat{\mathbf{y}} - c z_4 \hat{\mathbf{z}}$	(4h)	Te II

## 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>* **30**, 840–843 (1991), doi:10.1002/anie.199108401.
- [2] 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–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.

## Found in

- [1] P. Villars, *Ta<sub>2</sub>Ni<sub>2</sub>Te<sub>4</sub> (TaNiTe<sub>2</sub>) Crystal Structure* (2016). PAULING FILE in: *Inorganic Solid Phases*, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.