$TaNiTe_2$ Structure: ABC2_oP16_53_h_e_gh-001

This structure previously used the label(s) `ABC2_oP16_53_h_e_gh`. Calls to these addresses will be redirected here.

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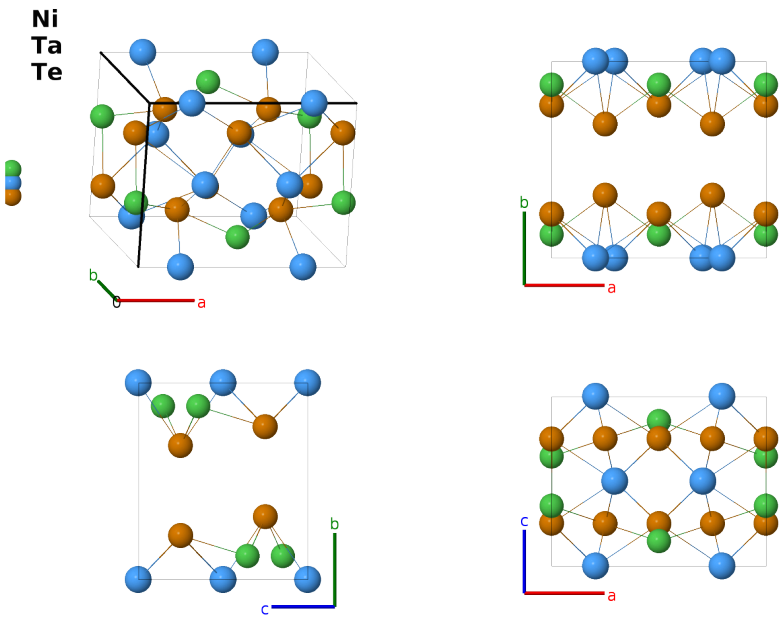
https://aflow.org/prototype-encyclopedia/AVNP

https://aflow.org/prototype-encyclopedia/ABC2_oP16_53_h_e_gh-001



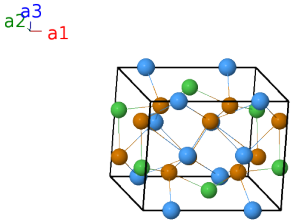
Prototype	$NiTaTe_2$
AFLOW prototype label	ABC2_oP16_53_h_e_gh-001
ICSD	71063
CCDC	1631976
Pearson symbol	oP16
Space group number	53
Space group symbol	*Pmna*
AFLOW prototype command	`aflow --proto=ABC2_oP16_53_h_e_gh-001 --params=`$a, b/a, c/a, x_1, y_2, y_3, z_3, y_4, z_4$

- Our original published version of this structure (Hicks, 2019) has incorrect lattice parameters. These are corrected here, and now show the layered structure of $TaNiTe_2$.

- 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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1$	=	$ax_1\,\hat{\mathbf{x}}$	(4e)	Ta I
$\mathbf{B_2}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4e)	Ta I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1$	=	$-ax_1\,\hat{\mathbf{x}}$	(4e)	Ta I
$\mathbf{B_4}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4e)	Ta I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1+y_2\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}+by_2\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(4g)	Te I
$\mathbf{B_6}$	=	$\frac{1}{4}\,\mathbf{a}_1-y_2\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}-by_2\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(4g)	Te I
$\mathbf{B_7}$	=	$\frac{3}{4}\,\mathbf{a}_1-y_2\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}}-by_2\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(4g)	Te I
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1+y_2\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}}+by_2\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(4g)	Te I
$\mathbf{B_9}$	=	$y_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(4h)	Ni I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1-y_3\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-by_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4h)	Ni I
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1+y_3\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+by_3\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4h)	Ni I
$\mathbf{B_{12}}$	=	$-y_3\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}}$	(4h)	Ni I
$\mathbf{B_{13}}$	=	$y_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(4h)	Te II
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_1-y_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4h)	Te II
$\mathbf{B_{15}}$	=	$\frac{1}{2}\,\mathbf{a}_1+y_4\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4h)	Te II
$\mathbf{B_{16}}$	=	$-y_4\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(4h)	Te II

References

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[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.

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First cited in

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