

NiNbTe₂ Structure:

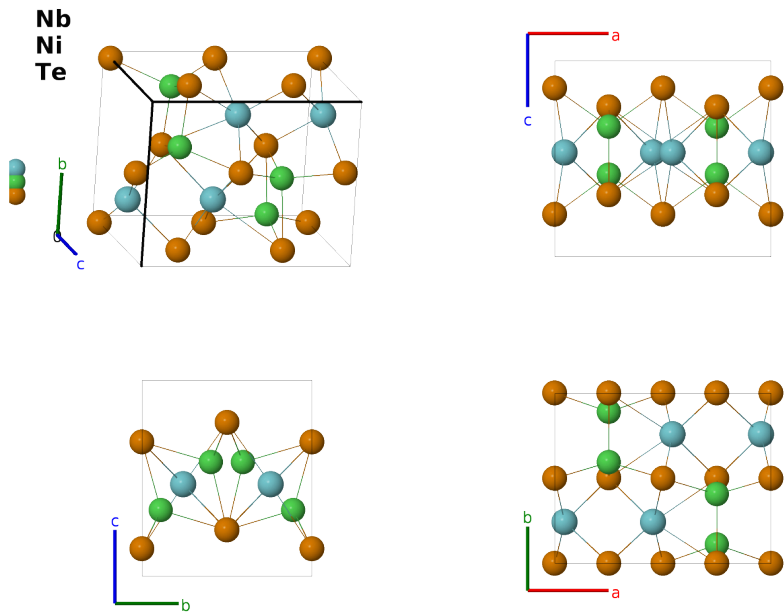
ABC2_oP16_28_d_2c_ab2c-001

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<https://aflow.org/prototype-encyclopedia/1GN1>

https://aflow.org/prototype-encyclopedia/ABC2_oP16_28_d_2c_ab2c-001



Prototype	NbNiTe ₂
AFLOW prototype label	ABC2_oP16_28_d_2c_ab2c-001
ICSD	71841
CCDC	632724
Pearson symbol	oP16
Space group number	28
Space group symbol	<i>Pma</i> 2
AFLOW prototype command	<code>aflow --proto=ABC2_oP16_28_d_2c_ab2c-001</code> <code>--params=a, b/a, c/a, z₁, z₂, y₃, z₃, y₄, z₄, y₅, z₅, y₆, z₆, x₇, y₇, z₇</code>

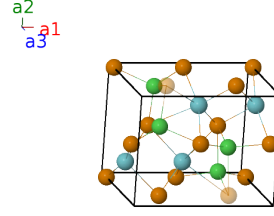
Other compounds with this structure

NiTaTe₂

- This is one of the few structures in the Encyclopedia where atoms are on all Wyckoff sites of the space group.

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
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(2a)	Te I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + cz_1 \hat{\mathbf{z}}$	(2a)	Te I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2b)	Te II
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2b)	Te II
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2c)	Ni I
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2c)	Ni I
$\mathbf{B}_7$	$= \frac{1}{4} \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2c)	Ni II
$\mathbf{B}_8$	$= \frac{3}{4} \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2c)	Ni II
$\mathbf{B}_9$	$= \frac{1}{4} \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(2c)	Te III
$\mathbf{B}_{10}$	$= \frac{3}{4} \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(2c)	Te III
$\mathbf{B}_{11}$	$= \frac{1}{4} \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(2c)	Te IV
$\mathbf{B}_{12}$	$= \frac{3}{4} \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(2c)	Te IV
$\mathbf{B}_{13}$	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4d)	Nb I
$\mathbf{B}_{14}$	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4d)	Nb I
$\mathbf{B}_{15}$	$= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4d)	Nb I
$\mathbf{B}_{16}$	$= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4d)	Nb I

References

- [1] J.-L. Huang, S.-X. Liu, and B.-Q. Huang, *Metal Clusters Synthesized by Solid State Reaction – Preparation and Crystal Structure of Two Mixed Metal Clusters, $\text{Ni}_2\text{Nb}_2\text{Te}_4(\text{I})$ AND $\text{Ni}_2\text{Ta}_2\text{Te}_4(\text{II})$* , Sci. China (Series B) **34**, 666–674 (1991), doi:10.1360/yb1991-34-6-666.

Found in

- [1] *Inorganic Crystal Structure Database*. Entry 71841 ($\text{Ni}_2\text{Nb}_2\text{Te}_4$).

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