

NbNiTe₅ Structure:

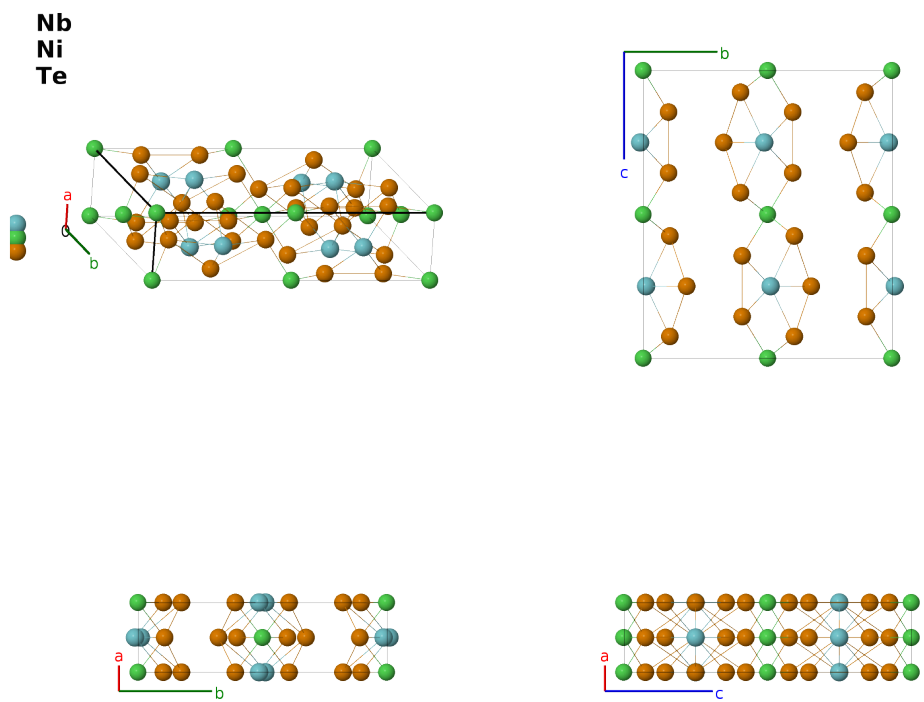
ABC5_oC28_63_c_a_c2f-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/BN2Z>

https://aflow.org/prototype-encyclopedia/ABC5_oC28_63_c_a_c2f-001



Prototype	NbNiTe ₅
AFLOW prototype label	ABC5_oC28_63_c_a_c2f-001
ICSD	73316
CCDC	1634128
Pearson symbol	oC28
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=ABC5_oC28_63_c_a_c2f-001</code> <code>--params=a, b/a, c/a, y₂, y₃, y₄, z₄, y₅, z₅</code>

Other compounds with this structure

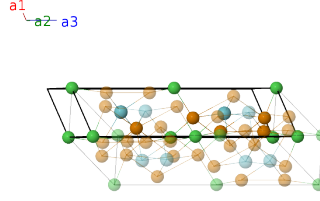
LaMgTe₅, TaNiTe₅, TaPtTe₅

Base-centered Orthorhombic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}$$

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(4a) Ni I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} c \hat{\mathbf{z}}$	(4a) Ni I
$\mathbf{B}_3$	=	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$by_2 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c) Nb I
$\mathbf{B}_4$	=	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$-by_2 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c) Nb I
$\mathbf{B}_5$	=	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$by_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c) Te I
$\mathbf{B}_6$	=	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$-by_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c) Te I
$\mathbf{B}_7$	=	$-y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8f) Te II
$\mathbf{B}_8$	=	$y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$-by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f) Te II
$\mathbf{B}_9$	=	$-y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	=	$by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f) Te II
$\mathbf{B}_{10}$	=	$y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8f) Te II
$\mathbf{B}_{11}$	=	$-y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8f) Te III
$\mathbf{B}_{12}$	=	$y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$-by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f) Te III
$\mathbf{B}_{13}$	=	$-y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	=	$by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f) Te III
$\mathbf{B}_{14}$	=	$y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8f) Te III

References

- [1] E. W. Liimatta and J. A. Ibers, *Synthesis, structure, and physical properties of the new layered ternary chalcogenide NbNiTe₅*, J. Solid State Chem. **71**, 384–389 (1987), doi:10.1016/0022-4596(87)90246-5.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.