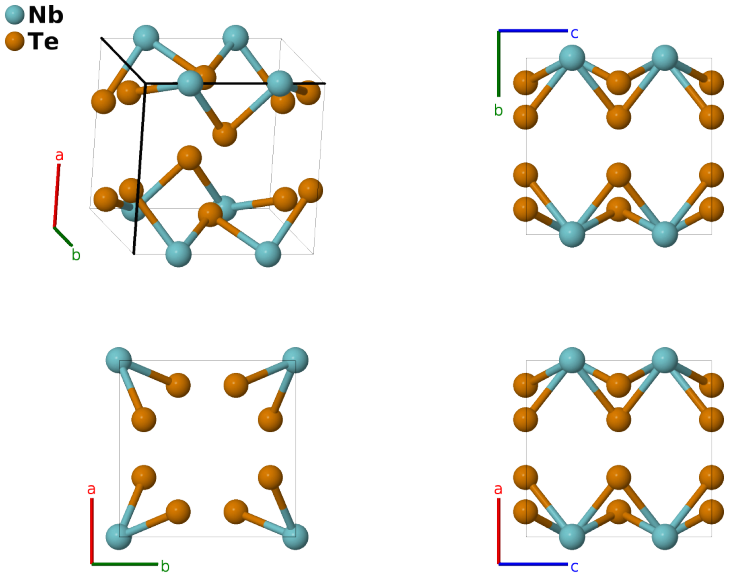
Room Temperature $NbTe_4$ Structure: AB4_tP10_124_a_m-001

This structure originally had the label `AB4_tP10_124_a_m`. Calls to that address will be redirected here.

Cite this page as: 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 (2019). doi: 10.1016/j.commatsci.2018.10.043

https://aflow.org/p/XFHX

https://aflow.org/p/AB4_tP10_124_a_m-001



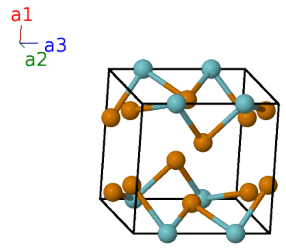
Prototype	$NbTe_4$
AFLOW prototype label	AB4_tP10_124_a_m-001
ICSD	43282
Pearson symbol	tP10
Space group number	124
Space group symbol	$P4/mcc$
AFLOW prototype command	`aflow --proto=AB4_tP10_124_a_m-001 --params=`$a, c/a, x_2, y_2$

Other compounds with this structure
$TaTe_4$

- This is the room-temperature phase of $NbTe4_4$. Above 520°C it transforms into a non-centrosymmetric structure.

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(2a)	Nb I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(2a)	Nb I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}}$	(8m)	Te I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}}$	(8m)	Te I
$\mathbf{B_5}$	=	$-y_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$-ay_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(8m)	Te I
$\mathbf{B_6}$	=	$y_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$ay_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(8m)	Te I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8m)	Te I
$\mathbf{B_8}$	=	$x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8m)	Te I
$\mathbf{B_9}$	=	$y_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8m)	Te I
$\mathbf{B_{10}}$	=	$-y_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8m)	Te I

References

[1] K. Selte and A. Kjekshus, *On the Crystal Structure of $NbTe_4$*, Acta Chem. Scand. **18**, 690–696 (1964), doi:10.3891/acta.chem.scand.18-0690.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.