High Temperature $NbTe_4$ Structure: AB4_tP10_103_a_d-001

This structure originally had the label `AB4_tP10_103_a_d`. Calls to that address will be redirected here.

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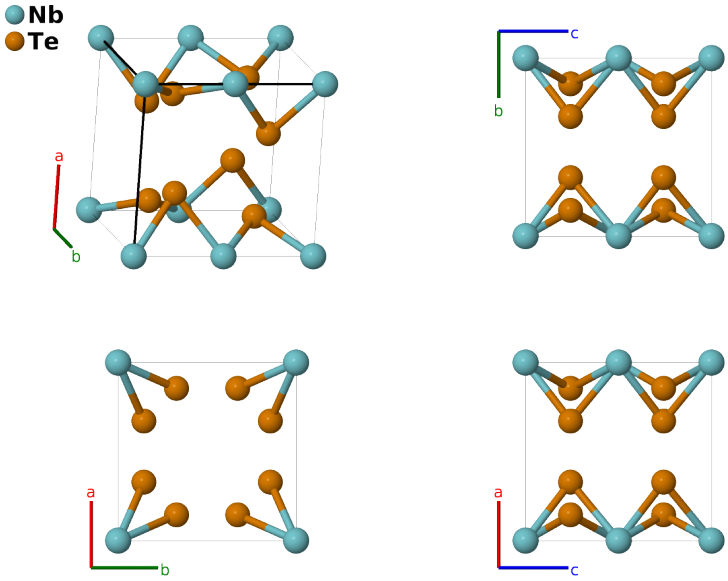
https://aflow.org/p/MRXL

https://aflow.org/p/AB4_tP10_103_a_d-001



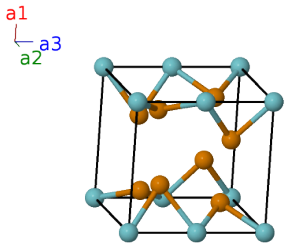
Prototype	$NbTe_4$
AFLOW prototype label	AB4_tP10_103_a_d-001
ICSD	65129
Pearson symbol	tP10
Space group number	103
Space group symbol	*P*4*cc*
AFLOW prototype command	`aflow --proto=AB4_tP10_103_a_d-001 --params=`$a, c/a, z_1, x_2, y_2, z_2$

Other compounds with this structure
$TaTe_4$

- This is the high-temperature phase of $NbTe_4$. Below 520°C it transforms into a centrosymmetric structure.
- Space group *P*4*cc* #103 has no inversion site and allows an arbitary origin for the z-axis. We fix this by setting $z_1 = 0$ for the niobium site.

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
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Nb I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Nb I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1+y_2\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}+ay_2\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(8d)	Te I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1-y_2\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}-ay_2\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(8d)	Te I
$\mathbf{B_5}$	=	$-y_2\,\mathbf{a}_1+x_2\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}}+ax_2\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(8d)	Te I
$\mathbf{B_6}$	=	$y_2\,\mathbf{a}_1-x_2\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}}-ax_2\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(8d)	Te I
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1-y_2\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}-ay_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Te I
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a}_1+y_2\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}+ay_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Te I
$\mathbf{B_9}$	=	$-y_2\,\mathbf{a}_1-x_2\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}}-ax_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Te I
$\mathbf{B_{10}}$	=	$y_2\,\mathbf{a}_1+x_2\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}}+ax_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	Te I

References

[1] H. Böhm, *The high temperature modification of niobium tetratelluride $NbTe_4$*, Z. Kristallogr. **180**, 113–122 (1987), doi:10.1524/zkri.1987.180.14.113.

Found in

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