$NbTe_2$ Structure: AB2_mC18_12_ai_3i-002

This structure originally had the label `AB2_mC18_12_ai_3i`. Calls to that address will be redirected here.

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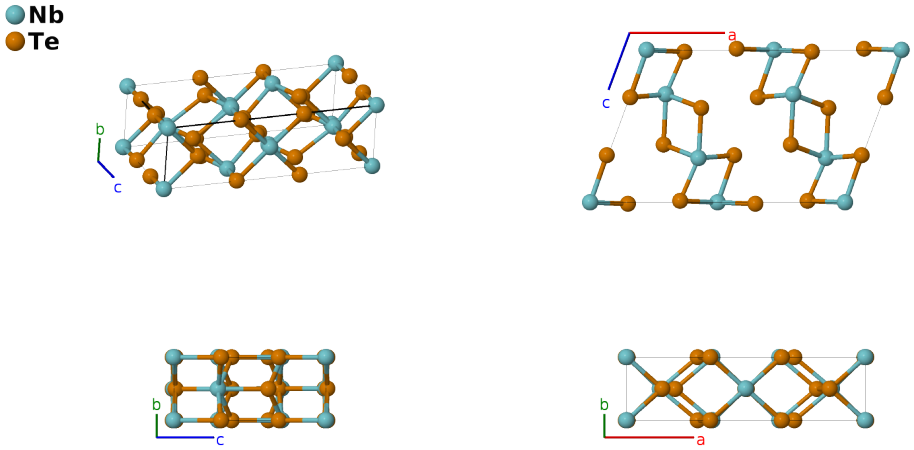
https://aflow.org/p/FY6X

https://aflow.org/p/AB2_mC18_12_ai_3i-002



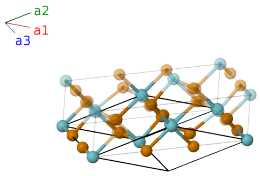
Prototype	$NbTe_2$
AFLOW prototype label	AB2_mC18_12_ai_3i-002
ICSD	14389
Pearson symbol	mC18
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=AB2_mC18_12_ai_3i-002 --params=`$a, b/a, c/a, \beta, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5$

Other compounds with this structure
$TaTe_2$, VTe_2

- FINDSYM found a somewhat more compact representation of the unit cell (smaller a and β) than that given in (Brown, 1966), so the lattice constants and Wyckoff parameters differ from those given in the reference.

Base-centered Monoclinic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Nb I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Nb II
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Nb II
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Te I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Te I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Te II
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Te II
$\mathbf{B_8}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Te III
$\mathbf{B_9}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Te III

References

[1] B. E. Brown, *The Crystal Structures of $NbTe_2$ and $TaTe_2$*, Acta Cryst. **20**, 264–267 (1966), doi:10.1107/S0365110X66000501.

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.