NbPS Structure: ABC_oI12_71_e_h_f-001

This structure previously used the label(s) `ABC_oI12_71_h_j_g`. Calls to these addresses will be redirected here.

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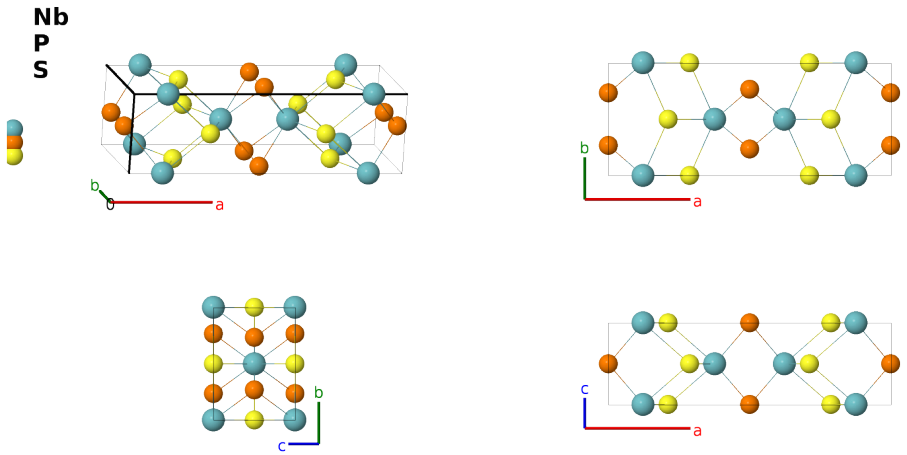
https://aflow.org/prototype-encyclopedia/B529

https://aflow.org/prototype-encyclopedia/ABC_oI12_71_e_h_f-001

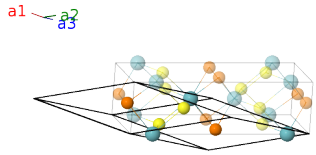


Prototype	NbPS
AFLOW prototype label	ABC_oI12_71_e_h_f-001
ICSD	16075
CCDC	1596724
Pearson symbol	oI12
Space group number	71
Space group symbol	$Immm$
AFLOW prototype command	`aflow --proto=ABC_oI12_71_e_h_f-001 --params=`$a, b/a, c/a, x_1, x_2, y_3$

- The ICSD lists this as a tenary form of UTe_2, but the structures are actually rather far apart.

Body-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}}$	(4e)	Nb I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}}$	(4e)	Nb I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(4f)	S I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(4f)	S I
$\mathbf{B_5}$	=	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	P I
$\mathbf{B_6}$	=	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	P I

References

[1] P. C. Donohue and P. E. Bierstedt, *Synthesis, crystal structure, and superconducting properties of niobium phosphorus sulfide, niobium phosphorus selenide and tantalum phosphorus sulfide*, Inorg. Chem. **8**, 2690–2694 (1969), doi:10.1021/ic50082a031.

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