

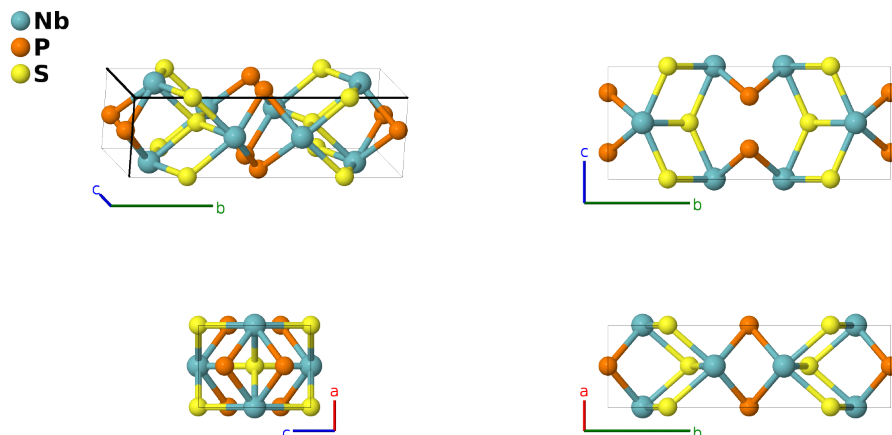
# NbPS Structure: ABC\_oI12\_71\_e\_h\_f-001

This structure originally had the label ABC\_oI12\_71\_h\_j\_g. Calls to that address will be redirected here.

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<https://aflow.org/p/B529>

[https://aflow.org/p/ABC\\_oI12\\_71\\_e\\_h\\_f-001](https://aflow.org/p/ABC_oI12_71_e_h_f-001)

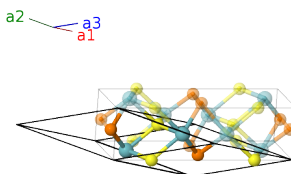


Prototype	NbPS
AFLOW prototype label	ABC_oI12_71_e_h_f-001
ICSD	16075
Pearson symbol	oI12
Space group number	71
Space group symbol	<i>I</i> mmm
AFLOW prototype command	aflow --proto=ABC_oI12_71_e_h_f-001 --params= <i>a</i> , <i>b/a</i> , <i>c/a</i> , <i>x</i> <sub>1</sub> , <i>x</i> <sub>2</sub> , <i>y</i> <sub>3</sub>

- The ICSD lists this as a ternary form of UTe<sub>2</sub>, but the structures are actually rather far apart.

## Body-centered Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}} \end{aligned}$$



## 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
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_1 + x_2 \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}$	(4f) S I
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 - x_2 \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}$	(4f) S I
$\mathbf{B}_5$	$=$	$(y_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h) P I
$\mathbf{B}_6$	$=$	$-(y_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(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.