Nb_4CoSi Structure: AB4C_tP12_124_a_m_c-001

This structure originally had the label `AB4C_tP12_124_a_m_c`. Calls to that address will be redirected here.

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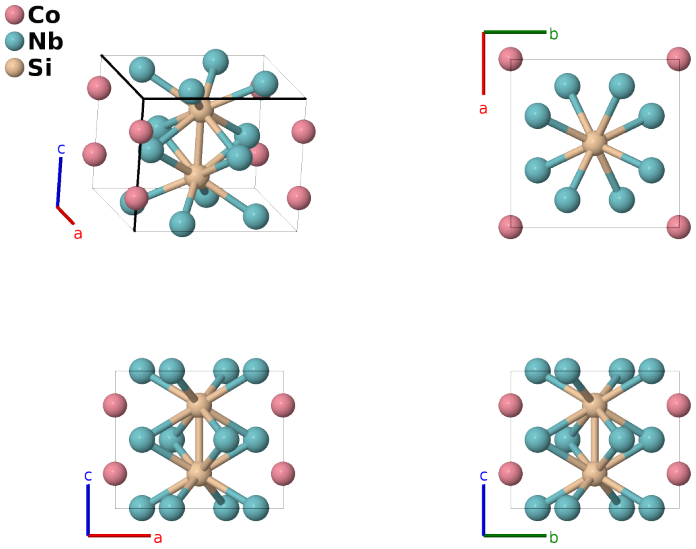
https://aflow.org/p/LAN3

https://aflow.org/p/AB4C_tP12_124_a_m_c-001

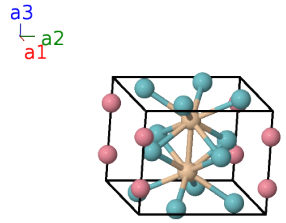


Prototype	$CoNb_4Si$
AFLOW prototype label	AB4C_tP12_124_a_m_c-001
ICSD	43233
Pearson symbol	tP12
Space group number	124
Space group symbol	$P4/mcc$
AFLOW prototype command	`aflow --proto=AB4C_tP12_124_a_m_c-001 --params=`$a, c/a, x_3, y_3$

Other compounds with this structure
Nb_4FeSi, Nb_4NiSi

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)	Co I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(2a)	Co I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Si I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Si I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}}$	(8m)	Nb I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}}$	(8m)	Nb I
$\mathbf{B_7}$	=	$-y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(8m)	Nb I
$\mathbf{B_8}$	=	$y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(8m)	Nb I
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8m)	Nb I
$\mathbf{B_{10}}$	=	$x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8m)	Nb I
$\mathbf{B_{11}}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8m)	Nb I
$\mathbf{B_{12}}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8m)	Nb I

References

[1] E. I. Gladyshevskii and Y. B. Kuz'ma, *The compounds Nb_4FeSi, Nb_4CoSi, Nb_4NiSi and their crystal structures*, J. Struct. Chem. **6** (1965), doi:10.1007/BF00743870.

Found in

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