Nb_6Sn_5 Structure: A6B5_oI44_71_egkl_fghl-001

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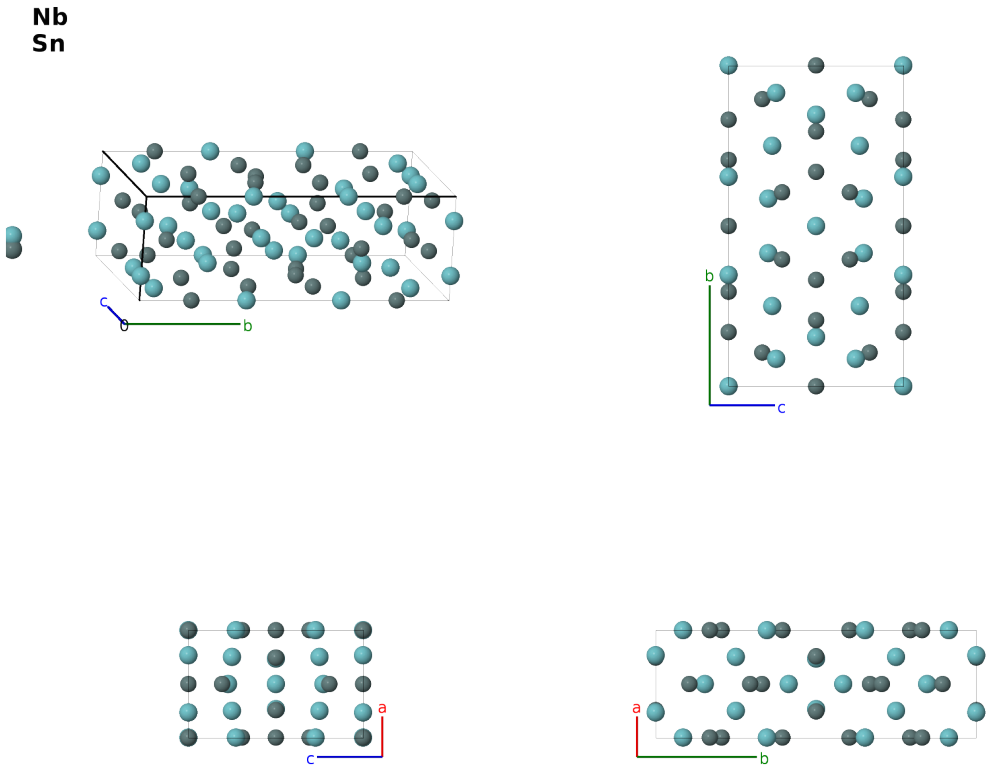
https://aflow.org/prototype-encyclopedia/Q45R

https://aflow.org/prototype-encyclopedia/A6B5_oI44_71_egkl_fghl-001



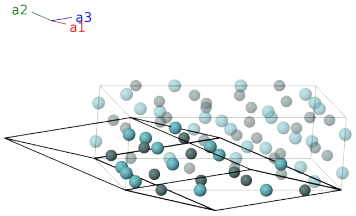
Prototype	Nb_6Sn_5
AFLOW prototype label	A6B5_oI44_71_egkl_fghl-001
ICSD	105232
CCDC	1663122
Pearson symbol	oI44
Space group number	71
Space group symbol	$Immm$
AFLOW prototype command	`aflow --proto=A6B5_oI44_71_egkl_fghl-001 --params=`$a, b/a, c/a, x_1, x_2, y_3, y_4, y_5, y_7, z_7, y_8, z_8$

Other compounds with this structure
Ti_6Sn_5

- (Ogren, 1965) state that what we have labeled the Sn-II (4g) site is only occupied 92% of the time.
- (Villars, 2018) and others use Ti_6Sn_5 as the prototype for this structure. We follow (Pearson, 1967) and use Nb_6Sn_5 as the prototype.

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)	Sn 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)	Sn I
$\mathbf{B_5}$	=	$y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}}$	(4g)	Nb II
$\mathbf{B_6}$	=	$-y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}}$	(4g)	Nb II
$\mathbf{B_7}$	=	$y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}}$	(4g)	Sn II
$\mathbf{B_8}$	=	$-y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}}$	(4g)	Sn II
$\mathbf{B_9}$	=	$\left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + y_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Sn III
$\mathbf{B_{10}}$	=	$-\left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - y_5\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Sn III
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8k)	Nb III
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - \frac{1}{4}c\,\hat{\mathbf{z}}$	(8k)	Nb III
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8k)	Nb III
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8k)	Nb III
$\mathbf{B_{15}}$	=	$(y_7 + z_7)\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + y_7\,\mathbf{a}_3$	=	$by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8l)	Nb IV
$\mathbf{B_{16}}$	=	$-(y_7 - z_7)\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 - y_7\,\mathbf{a}_3$	=	$-by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8l)	Nb IV
$\mathbf{B_{17}}$	=	$(y_7 - z_7)\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 + y_7\,\mathbf{a}_3$	=	$by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8l)	Nb IV
$\mathbf{B_{18}}$	=	$-(y_7 + z_7)\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 - y_7\,\mathbf{a}_3$	=	$-by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8l)	Nb IV
$\mathbf{B_{19}}$	=	$(y_8 + z_8)\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + y_8\,\mathbf{a}_3$	=	$by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8l)	Sn IV
$\mathbf{B_{20}}$	=	$-(y_8 - z_8)\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 - y_8\,\mathbf{a}_3$	=	$-by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8l)	Sn IV
$\mathbf{B_{21}}$	=	$(y_8 - z_8)\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 + y_8\,\mathbf{a}_3$	=	$by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(8l)	Sn IV

$$\mathbf{B_{22}} = -(y_8 + z_8)\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 - y_8\,\mathbf{a}_3 = -by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad (8l) \quad \text{Sn IV}$$

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