Foordite ($SnNb_2O_6$) Structure: A2B6C_mC36_15_f_3f_e-001

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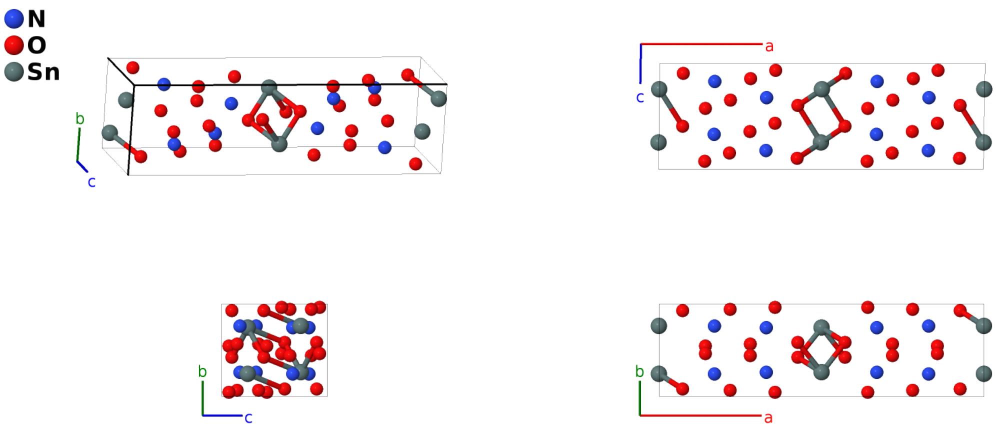
https://aflow.org/p/6QBH

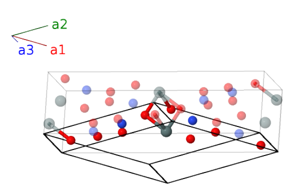
https://aflow.org/p/A2B6C_mC36_15_f_3f_e-001



Prototype	Nb_2O_6Sn
AFLOW prototype label	A2B6C_mC36_15_f_3f_e-001
Mineral name	foordite
ICSD	202827
Pearson symbol	mC36
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	`aflow --proto=A2B6C_mC36_15_f_3f_e-001` `--params=`$a, b/a, c/a, \beta, y_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Sn I

$\mathbf{B_{2}}$	$=$	$y_{1}\,\mathbf{a}_{1} - y_{1}\,\mathbf{a}_{2} + \frac{3}{4}\,\mathbf{a}_{3}$	$=$	$\frac{3}{4}c\cos\beta\,\mathbf{\hat{x}} - by_{1}\,\mathbf{\hat{y}} + \frac{3}{4}c\sin\beta\,\mathbf{\hat{z}}$	(4e)	Sn I
$\mathbf{B_{3}}$	$=$	$\left(x_{2} - y_{2}\right)\,\mathbf{a}_{1} + \left(x_{2} + y_{2}\right)\,\mathbf{a}_{2} + z_{2}\,\mathbf{a}_{3}$	$=$	$\left(ax_{2} + cz_{2}\cos\beta\right)\,\mathbf{\hat{x}} + by_{2}\,\mathbf{\hat{y}} + cz_{2}\sin\beta\,\mathbf{\hat{z}}$	(8f)	N I
$\mathbf{B_{4}}$	$=$	$-\left(x_{2} + y_{2}\right)\,\mathbf{a}_{1} - \left(x_{2} - y_{2}\right)\,\mathbf{a}_{2} - \left(z_{2} - \frac{1}{2}\right)\,\mathbf{a}_{3}$	$=$	$-\left(ax_{2} + c\left(z_{2} - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_{2}\,\mathbf{\hat{y}} - c\left(z_{2} - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	N I
$\mathbf{B_{5}}$	$=$	$-\left(x_{2} - y_{2}\right)\,\mathbf{a}_{1} - \left(x_{2} + y_{2}\right)\,\mathbf{a}_{2} - z_{2}\,\mathbf{a}_{3}$	$=$	$-\left(ax_{2} + cz_{2}\cos\beta\right)\,\mathbf{\hat{x}} - by_{2}\,\mathbf{\hat{y}} - cz_{2}\sin\beta\,\mathbf{\hat{z}}$	(8f)	N I
$\mathbf{B_{6}}$	$=$	$\left(x_{2} + y_{2}\right)\,\mathbf{a}_{1} + \left(x_{2} - y_{2}\right)\,\mathbf{a}_{2} + \left(z_{2} + \frac{1}{2}\right)\,\mathbf{a}_{3}$	$=$	$\left(ax_{2} + c\left(z_{2} + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_{2}\,\mathbf{\hat{y}} + c\left(z_{2} + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	N I
$\mathbf{B_{7}}$	$=$	$\left(x_{3} - y_{3}\right)\,\mathbf{a}_{1} + \left(x_{3} + y_{3}\right)\,\mathbf{a}_{2} + z_{3}\,\mathbf{a}_{3}$	$=$	$\left(ax_{3} + cz_{3}\cos\beta\right)\,\mathbf{\hat{x}} + by_{3}\,\mathbf{\hat{y}} + cz_{3}\sin\beta\,\mathbf{\hat{z}}$	(8f)	O I
$\mathbf{B_{8}}$	$=$	$-\left(x_{3} + y_{3}\right)\,\mathbf{a}_{1} - \left(x_{3} - y_{3}\right)\,\mathbf{a}_{2} - \left(z_{3} - \frac{1}{2}\right)\,\mathbf{a}_{3}$	$=$	$-\left(ax_{3} + c\left(z_{3} - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_{3}\,\mathbf{\hat{y}} - c\left(z_{3} - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O I
$\mathbf{B_{9}}$	$=$	$-\left(x_{3} - y_{3}\right)\,\mathbf{a}_{1} - \left(x_{3} + y_{3}\right)\,\mathbf{a}_{2} - z_{3}\,\mathbf{a}_{3}$	$=$	$-\left(ax_{3} + cz_{3}\cos\beta\right)\,\mathbf{\hat{x}} - by_{3}\,\mathbf{\hat{y}} - cz_{3}\sin\beta\,\mathbf{\hat{z}}$	(8f)	O I
$\mathbf{B_{10}}$	$=$	$\left(x_{3} + y_{3}\right)\,\mathbf{a}_{1} + \left(x_{3} - y_{3}\right)\,\mathbf{a}_{2} + \left(z_{3} + \frac{1}{2}\right)\,\mathbf{a}_{3}$	$=$	$\left(ax_{3} + c\left(z_{3} + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_{3}\,\mathbf{\hat{y}} + c\left(z_{3} + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O I
$\mathbf{B_{11}}$	$=$	$\left(x_{4} - y_{4}\right)\,\mathbf{a}_{1} + \left(x_{4} + y_{4}\right)\,\mathbf{a}_{2} + z_{4}\,\mathbf{a}_{3}$	$=$	$\left(ax_{4} + cz_{4}\cos\beta\right)\,\mathbf{\hat{x}} + by_{4}\,\mathbf{\hat{y}} + cz_{4}\sin\beta\,\mathbf{\hat{z}}$	(8f)	O II
$\mathbf{B_{12}}$	$=$	$-\left(x_{4} + y_{4}\right)\,\mathbf{a}_{1} - \left(x_{4} - y_{4}\right)\,\mathbf{a}_{2} - \left(z_{4} - \frac{1}{2}\right)\,\mathbf{a}_{3}$	$=$	$-\left(ax_{4} + c\left(z_{4} - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_{4}\,\mathbf{\hat{y}} - c\left(z_{4} - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O II
$\mathbf{B_{13}}$	$=$	$-\left(x_{4} - y_{4}\right)\,\mathbf{a}_{1} - \left(x_{4} + y_{4}\right)\,\mathbf{a}_{2} - z_{4}\,\mathbf{a}_{3}$	$=$	$-\left(ax_{4} + cz_{4}\cos\beta\right)\,\mathbf{\hat{x}} - by_{4}\,\mathbf{\hat{y}} - cz_{4}\sin\beta\,\mathbf{\hat{z}}$	(8f)	O II
$\mathbf{B_{14}}$	$=$	$\left(x_{4} + y_{4}\right)\,\mathbf{a}_{1} + \left(x_{4} - y_{4}\right)\,\mathbf{a}_{2} + \left(z_{4} + \frac{1}{2}\right)\,\mathbf{a}_{3}$	$=$	$\left(ax_{4} + c\left(z_{4} + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_{4}\,\mathbf{\hat{y}} + c\left(z_{4} + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O II
$\mathbf{B_{15}}$	$=$	$\left(x_{5} - y_{5}\right)\,\mathbf{a}_{1} + \left(x_{5} + y_{5}\right)\,\mathbf{a}_{2} + z_{5}\,\mathbf{a}_{3}$	$=$	$\left(ax_{5} + cz_{5}\cos\beta\right)\,\mathbf{\hat{x}} + by_{5}\,\mathbf{\hat{y}} + cz_{5}\sin\beta\,\mathbf{\hat{z}}$	(8f)	O III
$\mathbf{B_{16}}$	$=$	$-\left(x_{5} + y_{5}\right)\,\mathbf{a}_{1} - \left(x_{5} - y_{5}\right)\,\mathbf{a}_{2} - \left(z_{5} - \frac{1}{2}\right)\,\mathbf{a}_{3}$	$=$	$-\left(ax_{5} + c\left(z_{5} - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_{5}\,\mathbf{\hat{y}} - c\left(z_{5} - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O III
$\mathbf{B_{17}}$	$=$	$-\left(x_{5} - y_{5}\right)\,\mathbf{a}_{1} - \left(x_{5} + y_{5}\right)\,\mathbf{a}_{2} - z_{5}\,\mathbf{a}_{3}$	$=$	$-\left(ax_{5} + cz_{5}\cos\beta\right)\,\mathbf{\hat{x}} - by_{5}\,\mathbf{\hat{y}} - cz_{5}\sin\beta\,\mathbf{\hat{z}}$	(8f)	O III
$\mathbf{B_{18}}$	$=$	$\left(x_{5} + y_{5}\right)\,\mathbf{a}_{1} + \left(x_{5} - y_{5}\right)\,\mathbf{a}_{2} + \left(z_{5} + \frac{1}{2}\right)\,\mathbf{a}_{3}$	$=$	$\left(ax_{5} + c\left(z_{5} + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_{5}\,\mathbf{\hat{y}} + c\left(z_{5} + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O III

References

[1] T. S. Ercit and P. Černý, *The Crystal Structure of Foordite*, Can. Mineral. **26**, 899–903 (1988).