

Foordite (SnNb₂O₆) Structure:

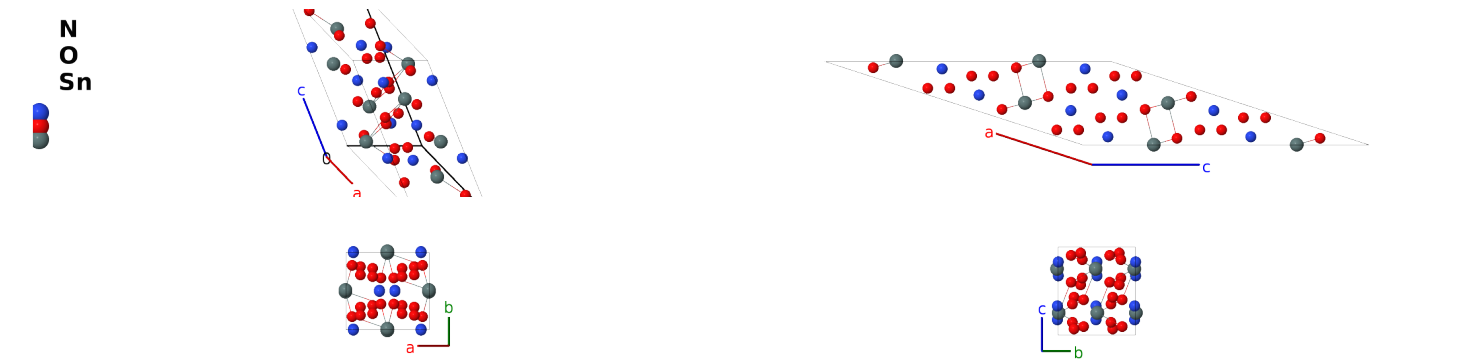
A2B6C_mC36_15_f_3f_e-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/6QBH>

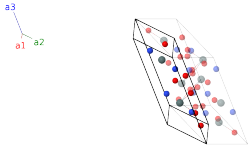
https://aflow.org/prototype-encyclopedia/A2B6C_mC36_15_f_3f_e-001



Prototype	Nb ₂ O ₆ Sn
AFLOW prototype label	A2B6C_mC36_15_f_3f_e-001
Mineral name	foordite
ICSD	202827
CCDC	1707391
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

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



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

$$\begin{aligned}
\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 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + \frac{3}{4} c \sin \beta \hat{\mathbf{z}} &(4e) &\text{Sn I} \\
\mathbf{B}_3 &= (x_2 - y_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3 &= (ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}} &(8f) &\text{N I} \\
\mathbf{B}_4 &= -(x_2 + y_2) \mathbf{a}_1 - (x_2 - y_2) \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) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(8f) &\text{N I} \\
\mathbf{B}_5 &= -(x_2 - y_2) \mathbf{a}_1 - (x_2 + y_2) \mathbf{a}_2 - z_2 \mathbf{a}_3 &= -(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}} &(8f) &\text{N I} \\
\mathbf{B}_6 &= (x_2 + y_2) \mathbf{a}_1 + (x_2 - y_2) \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) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(8f) &\text{N I} \\
\mathbf{B}_7 &= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3 &= (ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}} &(8f) &\text{O I} \\
\mathbf{B}_8 &= -(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \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) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(8f) &\text{O I} \\
\mathbf{B}_9 &= -(x_3 - y_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}} &(8f) &\text{O I} \\
\mathbf{B}_{10} &= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \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) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(8f) &\text{O I} \\
\mathbf{B}_{11} &= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3 &= (ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}} &(8f) &\text{O II} \\
\mathbf{B}_{12} &= -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \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) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(8f) &\text{O II} \\
\mathbf{B}_{13} &= -(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}} &(8f) &\text{O II} \\
\mathbf{B}_{14} &= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \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) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(8f) &\text{O II} \\
\mathbf{B}_{15} &= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3 &= (ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}} &(8f) &\text{O III} \\
\mathbf{B}_{16} &= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \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) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(8f) &\text{O III} \\
\mathbf{B}_{17} &= -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}} &(8f) &\text{O III} \\
\mathbf{B}_{18} &= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \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) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(8f) &\text{O III}
\end{aligned}$$

References

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

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.