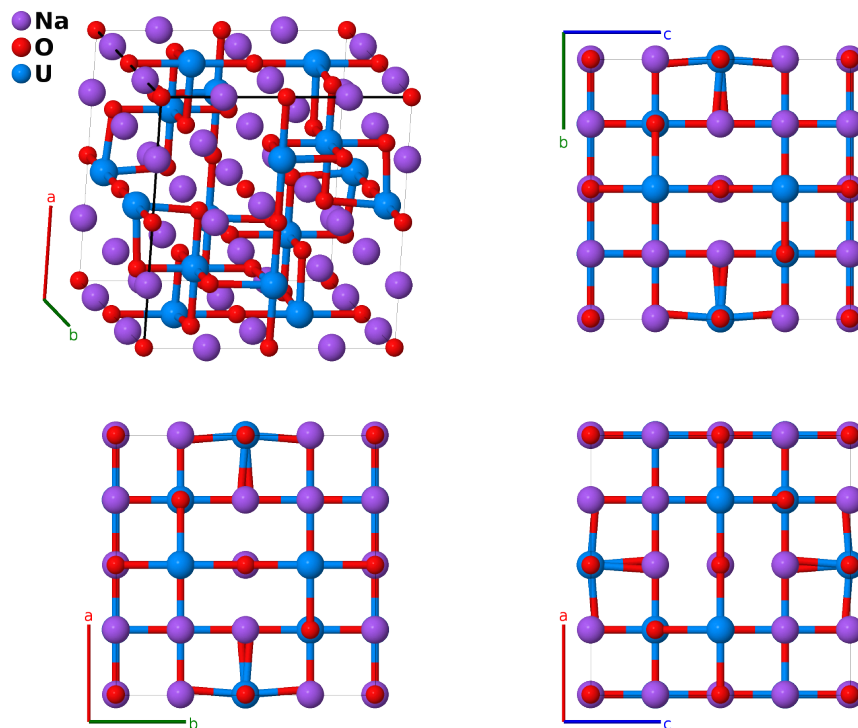


Na₁₁U₅O₁₆ Structure: A11B16C5_cP64_208_bfh_adm_ce-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

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

https://aflow.org/p/A11B16C5_cP64_208_bfh_adm_ce-001



Prototype	Na ₁₁ O ₁₆ U ₅
AFLOW prototype label	A11B16C5_cP64_208_bfh_adm_ce-001
ICSD	15137
Pearson symbol	cP64
Space group number	208
Space group symbol	<i>P</i> 4 ₂ 32
AFLOW prototype command	<code>aflow --proto=A11B16C5_cP64_208_bfh_adm_ce-001 --params=a, x₇, x₈, y₈, z₈</code>

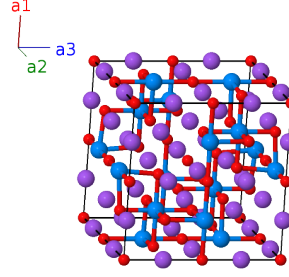
- (Bartram, 1970) say the atoms were “arbitrarily placed” at the Wyckoff positions listed, with $z_8 = 0$. This gives a U₁-O₃ distance of 2.38Å. They then set $z_8 = -0.02$ (0.52 using our origin), giving a distance of 2.19Å, which they consider “more reasonable,” but the other U-O distances remain at 2.39Å. If we find a refinement of this structure we will update this page.

Simple Cubic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(2a)	O I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(2a)	O I
\mathbf{B}_3	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(4b)	Na I
\mathbf{B}_4	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(4b)	Na I
\mathbf{B}_5	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(4b)	Na I
\mathbf{B}_6	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(4b)	Na I
\mathbf{B}_7	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(4c)	U I
\mathbf{B}_8	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(4c)	U I
\mathbf{B}_9	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(4c)	U I
\mathbf{B}_{10}	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(4c)	U I
\mathbf{B}_{11}	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6d)	O II
\mathbf{B}_{12}	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6d)	O II
\mathbf{B}_{13}	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6d)	O II
\mathbf{B}_{14}	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{y}}$	(6d)	O II
\mathbf{B}_{15}	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(6d)	O II
\mathbf{B}_{16}	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{z}}$	(6d)	O II
\mathbf{B}_{17}	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6e)	U II
\mathbf{B}_{18}	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6e)	U II
\mathbf{B}_{19}	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(6e)	U II
\mathbf{B}_{20}	$\frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(6e)	U II
\mathbf{B}_{21}	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(6e)	U II
\mathbf{B}_{22}	$\frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(6e)	U II
\mathbf{B}_{23}	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6f)	Na II
\mathbf{B}_{24}	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6f)	Na II
\mathbf{B}_{25}	$\frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f)	Na II
\mathbf{B}_{26}	$\frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f)	Na II
\mathbf{B}_{27}	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{z}}$	(6f)	Na II
\mathbf{B}_{28}	$\frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{z}}$	(6f)	Na II

$$\mathbf{B}_{62} = \begin{pmatrix} (z_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + \\ (x_8 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(z_8 + \frac{1}{2} \right) \hat{\mathbf{x}} - a \left(y_8 - \frac{1}{2} \right) \hat{\mathbf{y}} + a \left(x_8 + \frac{1}{2} \right) \hat{\mathbf{z}} \quad (24m) \quad \text{O III}$$

$$\mathbf{B}_{63} = \begin{pmatrix} -(z_8 - \frac{1}{2}) \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_8 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(z_8 - \frac{1}{2} \right) \hat{\mathbf{x}} + a \left(y_8 + \frac{1}{2} \right) \hat{\mathbf{y}} + a \left(x_8 + \frac{1}{2} \right) \hat{\mathbf{z}} \quad (24m) \quad \text{O III}$$

$$\mathbf{B}_{64} = \begin{pmatrix} -(z_8 - \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 - \\ (x_8 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(z_8 - \frac{1}{2} \right) \hat{\mathbf{x}} - a \left(y_8 - \frac{1}{2} \right) \hat{\mathbf{y}} - a \left(x_8 - \frac{1}{2} \right) \hat{\mathbf{z}} \quad (24m) \quad \text{O III}$$

References

- [1] S. F. Bartram and R. E. Fryxell, *Preparation and crystal structure of NaUO₃ and Na₁₁U₅O₁₆*, J. Inorg. Nucl. Chem. **32**, 3701–3706 (1970), doi:10.1016/0022-1902(70)80187-7.