

Bi₃Ru₃O₁₁ Structure: A3B11C3_cP68_201_be_efh_g-001

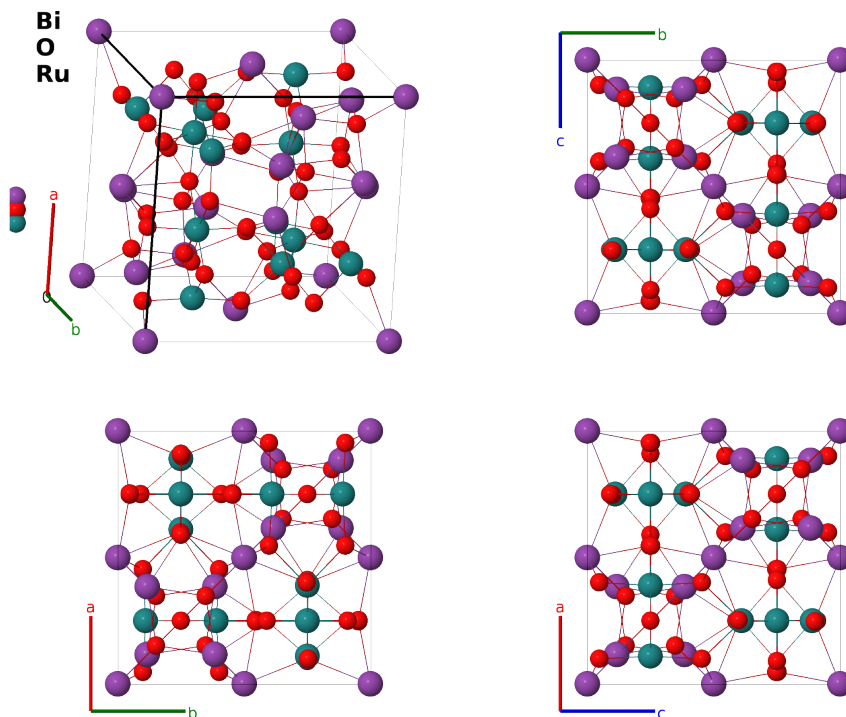
This structure previously used the label(s) **A3B11C3_cP68_201_be_efh_g**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/0WEU>

https://aflow.org/prototype-encyclopedia/A3B11C3_cP68_201_be_efh_g-001



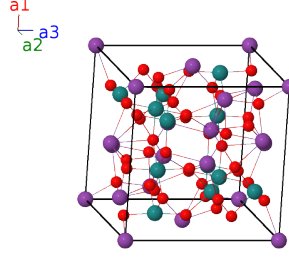
Prototype	Bi ₃ O ₁₁ Ru ₃
AFLOW prototype label	A3B11C3_cP68_201_be_efh_g-001
ICSD	4194
CCDC	1592879
Pearson symbol	cP68
Space group number	201
Space group symbol	$Pn\bar{3}$
AFLOW prototype command	<pre>aflow --proto=A3B11C3_cP68_201_be_efh_g-001 --params=a, x2, x3, x4, x5, x6, y6, z6</pre>

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	(4b) Bi I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(4b) Bi I
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4b) Bi I
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4b) Bi I
$\mathbf{B}_5$	$=$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8e) Bi II
$\mathbf{B}_6$	$=$	$-\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8e) Bi II
$\mathbf{B}_7$	$=$	$-\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + x_2 \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e) Bi II
$\mathbf{B}_8$	$=$	$x_2 \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e) Bi II
$\mathbf{B}_9$	$=$	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8e) Bi II
$\mathbf{B}_{10}$	$=$	$\left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8e) Bi II
$\mathbf{B}_{11}$	$=$	$\left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e) Bi II
$\mathbf{B}_{12}$	$=$	$-x_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e) Bi II
$\mathbf{B}_{13}$	$=$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(8e) O I
$\mathbf{B}_{14}$	$=$	$-\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(8e) O I
$\mathbf{B}_{15}$	$=$	$-\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e) O I
$\mathbf{B}_{16}$	$=$	$x_3 \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e) O I
$\mathbf{B}_{17}$	$=$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(8e) O I
$\mathbf{B}_{18}$	$=$	$\left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(8e) O I
$\mathbf{B}_{19}$	$=$	$\left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e) O I
$\mathbf{B}_{20}$	$=$	$-x_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e) O I
$\mathbf{B}_{21}$	$=$	$x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12f) O II
$\mathbf{B}_{22}$	$=$	$-\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12f) O II
$\mathbf{B}_{23}$	$=$	$\frac{1}{4} \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12f) O II
$\mathbf{B}_{24}$	$=$	$\frac{1}{4} \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12f) O II

$$\begin{aligned}
\mathbf{B}_{61} &= -z_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - y_6 \mathbf{a}_3 &= -az_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}} &(24h) &\text{O III} \\
\mathbf{B}_{62} &= -z_6 \mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_2 + &= -az_6 \hat{\mathbf{x}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(24h) &\text{O III} \\
&\quad \left(y_6 + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{63} &= \left(z_6 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_2 - y_6 \mathbf{a}_3 &= a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}} &(24h) &\text{O III} \\
\mathbf{B}_{64} &= \left(z_6 + \frac{1}{2}\right) \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_3 &= a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(24h) &\text{O III} \\
\mathbf{B}_{65} &= -y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 - x_6 \mathbf{a}_3 &= -ay_6 \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}} &(24h) &\text{O III} \\
\mathbf{B}_{66} &= \left(y_6 + \frac{1}{2}\right) \mathbf{a}_1 - z_6 \mathbf{a}_2 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_3 &= a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(24h) &\text{O III} \\
\mathbf{B}_{67} &= -y_6 \mathbf{a}_1 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_2 + &= -ay_6 \hat{\mathbf{x}} + a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{z}} &(24h) &\text{O III} \\
&\quad \left(x_6 + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{68} &= \left(y_6 + \frac{1}{2}\right) \mathbf{a}_1 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_2 - x_6 \mathbf{a}_3 &= a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}} &(24h) &\text{O III}
\end{aligned}$$

References

- [1] F. Abraham, D. Thomas, and G. Nowogrocki, *Structure cristalline de $\text{Bi}_3\text{Ru}_3\text{O}_{11}$* , Bull. Soc. fr. Minéral. Cristallogr. **98**, 25–29 (1975), doi:10.3406/bulmi.1975.6954.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

- 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.