

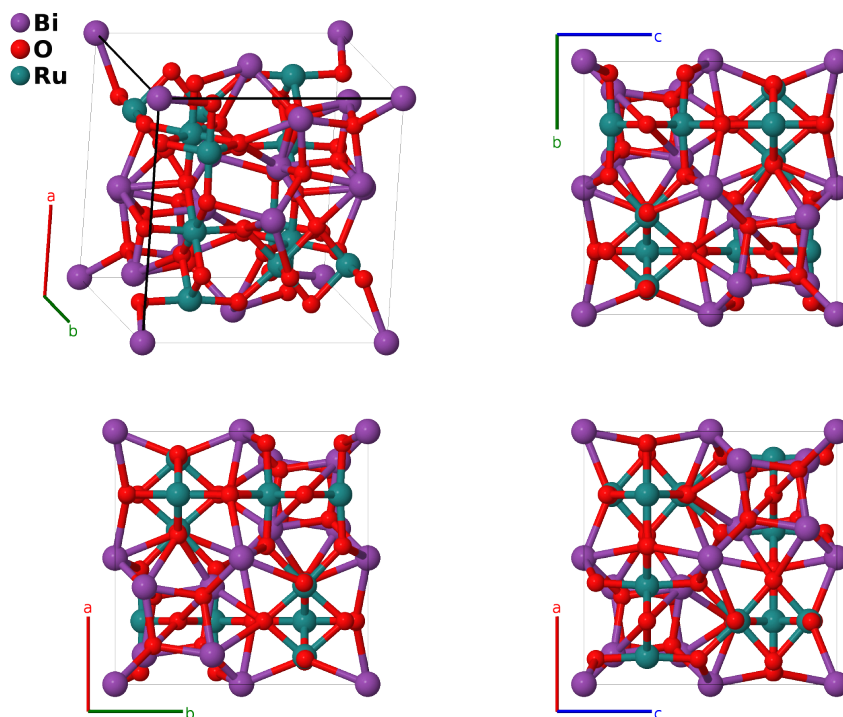
# Bi<sub>3</sub>Ru<sub>3</sub>O<sub>11</sub> Structure: A3B11C3\_cP68\_201\_be\_efh\_g-001

This structure originally had the label A3B11C3\_cP68\_201\_be\_efh\_g. Calls to that address will be redirected here.

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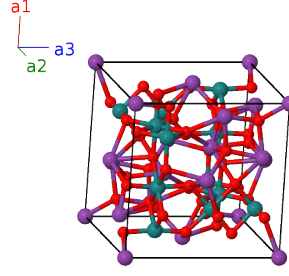
<https://aflow.org/p/0WEU>

[https://aflow.org/p/A3B11C3\\_cP68\\_201\\_be\\_efh\\_g-001](https://aflow.org/p/A3B11C3_cP68_201_be_efh_g-001)



Prototype	Bi <sub>3</sub> O <sub>11</sub> Ru <sub>3</sub>
AFLOW prototype label	A3B11C3_cP68_201_be_efh_g-001
ICSD	4194
Pearson symbol	cP68
Space group number	201
Space group symbol	$Pn\bar{3}$
AFLOW prototype command	<code>aflow --proto=A3B11C3_cP68_201_be_efh_g-001 --params=a, x<sub>2</sub>, x<sub>3</sub>, x<sub>4</sub>, x<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub></code>

Simple Cubic primitive vectors



$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}}\end{aligned}$$

## 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
$\mathbf{B}_6$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8e)	Bi II
$\mathbf{B}_7$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Bi II
$\mathbf{B}_8$	$x_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{10}$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8e)	Bi II
$\mathbf{B}_{11}$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Bi II
$\mathbf{B}_{12}$	$-x_2 \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{14}$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B}_{15}$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 - (x_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B}_{16}$	$x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 - (x_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{18}$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B}_{19}$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B}_{20}$	$-x_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{22}$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(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
$\mathbf{B}_{24}$	$\frac{1}{4} \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12f)	O II
$\mathbf{B}_{25}$	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(12f)	O II



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

## References

- [1] F. Abraham, D. Thomas, and G. Nowogrocki, *Structure cristalline de  $Bi_3Ru_3O_{11}$* , 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).