

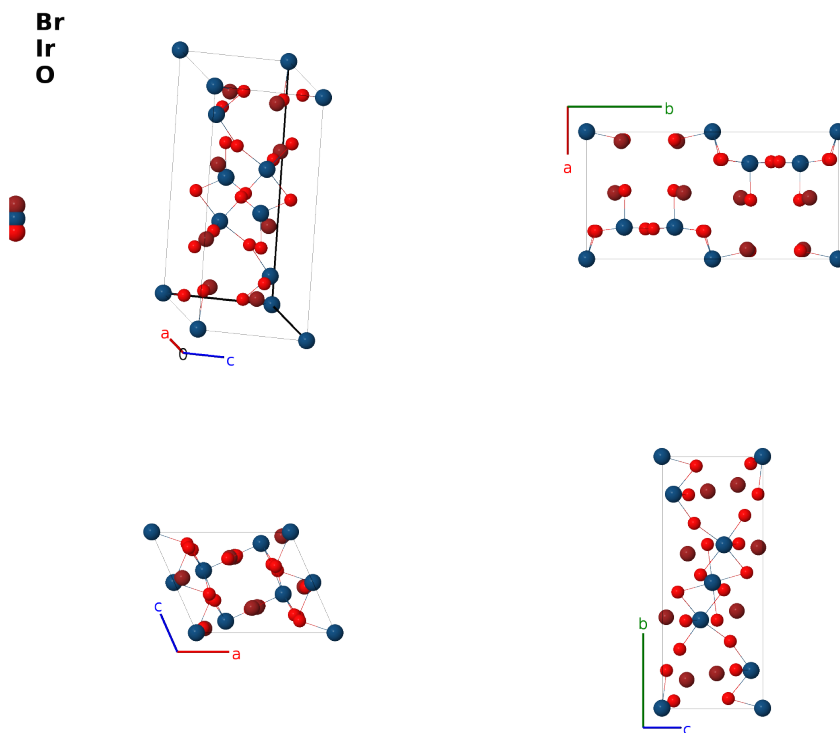
# Ba<sub>4</sub>Ir<sub>3</sub>O<sub>10</sub> Structure: A4B3C10\_mP34\_14\_2e\_ae\_5e-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, 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/7TLN>

[https://aflow.org/prototype-encyclopedia/A4B3C10\\_mP34\\_14\\_2e\\_ae\\_5e-001](https://aflow.org/prototype-encyclopedia/A4B3C10_mP34_14_2e_ae_5e-001)



|                         |                                                                                                                                                                                                                                           |
|-------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype               | Ba <sub>4</sub> Ir <sub>3</sub> O <sub>10</sub>                                                                                                                                                                                           |
| AFLOW prototype label   | A4B3C10_mP34_14_2e_ae_5e-001                                                                                                                                                                                                              |
| ICSD                    | 33863                                                                                                                                                                                                                                     |
| CCDC                    | 1606604                                                                                                                                                                                                                                   |
| Pearson symbol          | mP34                                                                                                                                                                                                                                      |
| Space group number      | 14                                                                                                                                                                                                                                        |
| Space group symbol      | $P2_1/c$                                                                                                                                                                                                                                  |
| AFLOW prototype command | <pre>aflow --proto=A4B3C10_mP34_14_2e_ae_5e-001       --params=a, b/a, c/a, <math>\beta</math>, <math>x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9</math></pre> |

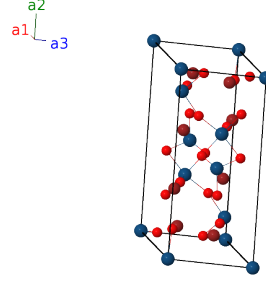
## Other compounds with this structure

Ba<sub>4</sub>Ru<sub>3</sub>O<sub>10</sub>

- (Wilkins, 1991) give the structure in the  $P2_1/a$  setting of space group #14. We used AFLOW to transform this to the standard  $P2_1/c$  setting. This essentially swaps the a and c vectors, with a small change in the length of the a vector and the angle  $\beta$ .

## Simple Monoclinic primitive vectors

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



## Basis vectors

|                   | Lattice coordinates                                                                       |     | Cartesian coordinates                                                                                                                                   | Wyckoff position | Atom type |
|-------------------|-------------------------------------------------------------------------------------------|-----|---------------------------------------------------------------------------------------------------------------------------------------------------------|------------------|-----------|
| $\mathbf{B}_1$    | $0$                                                                                       | $=$ | $0$                                                                                                                                                     | (2a)             | Ir I      |
| $\mathbf{B}_2$    | $\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$                                     | $=$ | $\frac{1}{2} c \cos \beta \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$                                | (2a)             | Ir I      |
| $\mathbf{B}_3$    | $x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$                                  | $=$ | $(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$                                                  | (4e)             | Br I      |
| $\mathbf{B}_4$    | $-x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-(ax_2 + c(z_2 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (4e)             | Br I      |
| $\mathbf{B}_5$    | $-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$                                 | $=$ | $-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$                                                 | (4e)             | Br I      |
| $\mathbf{B}_6$    | $x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$  | (4e)             | Br I      |
| $\mathbf{B}_7$    | $x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$                                  | $=$ | $(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$                                                  | (4e)             | Br II     |
| $\mathbf{B}_8$    | $-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (4e)             | Br II     |
| $\mathbf{B}_9$    | $-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$                                 | $=$ | $-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$                                                 | (4e)             | Br II     |
| $\mathbf{B}_{10}$ | $x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$  | (4e)             | Br II     |
| $\mathbf{B}_{11}$ | $x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$                                  | $=$ | $(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$                                                  | (4e)             | Ir II     |
| $\mathbf{B}_{12}$ | $-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (4e)             | Ir II     |
| $\mathbf{B}_{13}$ | $-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$                                 | $=$ | $-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$                                                 | (4e)             | Ir II     |
| $\mathbf{B}_{14}$ | $x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$  | (4e)             | Ir II     |
| $\mathbf{B}_{15}$ | $x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$                                  | $=$ | $(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$                                                  | (4e)             | O I       |
| $\mathbf{B}_{16}$ | $-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-(ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$ | (4e)             | O I       |
| $\mathbf{B}_{17}$ | $-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$                                 | $=$ | $-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$                                                 | (4e)             | O I       |

$$\begin{aligned}
\mathbf{B}_{18} &= x_5 \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} (ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - \\ b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4e) & \text{O I} \\
\mathbf{B}_{19} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = \begin{pmatrix} (ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4e) & \text{O II} \\
\mathbf{B}_{20} &= -x_6 \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} -(ax_6 + c(z_6 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + \\ b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4e) & \text{O II} \\
\mathbf{B}_{21} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 = \begin{pmatrix} -(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4e) & \text{O II} \\
\mathbf{B}_{22} &= x_6 \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} (ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - \\ b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4e) & \text{O II} \\
\mathbf{B}_{23} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = \begin{pmatrix} (ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4e) & \text{O III} \\
\mathbf{B}_{24} &= -x_7 \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} -(ax_7 + c(z_7 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + \\ b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4e) & \text{O III} \\
\mathbf{B}_{25} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 = \begin{pmatrix} -(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4e) & \text{O III} \\
\mathbf{B}_{26} &= x_7 \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} (ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - \\ b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4e) & \text{O III} \\
\mathbf{B}_{27} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = \begin{pmatrix} (ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4e) & \text{O IV} \\
\mathbf{B}_{28} &= -x_8 \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} -(ax_8 + c(z_8 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + \\ b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4e) & \text{O IV} \\
\mathbf{B}_{29} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 = \begin{pmatrix} -(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4e) & \text{O IV} \\
\mathbf{B}_{30} &= x_8 \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} (ax_8 + c(z_8 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - \\ b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4e) & \text{O IV} \\
\mathbf{B}_{31} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = \begin{pmatrix} (ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4e) & \text{O V} \\
\mathbf{B}_{32} &= -x_9 \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} -(ax_9 + c(z_9 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + \\ b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4e) & \text{O V} \\
\mathbf{B}_{33} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 = \begin{pmatrix} -(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4e) & \text{O V} \\
\mathbf{B}_{34} &= x_9 \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} (ax_9 + c(z_9 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - \\ b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} & (4e) & \text{O V}
\end{aligned}$$

## References

- [1] J. Wilkens and H. Müller-Buschbaum, *Zur Kenntnis von  $Ba_4Ir_3O_{10}$* , Z. Anorganische und Allgemeine Chemie **592**, 79–83 (1991), doi:10.1002/zaac.19915920109.

## Found in

- [1] C. Dussarrat, F. Grasset, R. Bontchev, and J. Darriet, *Crystal structures and magnetic properties of  $Ba_4Ru_3O_{10}$  and  $Ba_5Ru_3O_{12}$* , J. Alloys Compd. **233**, 15–22 (1996), doi:10.1016/0925-8388(96)80029-6.

## First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).