

Base-centered Orthorhombic $\text{Sr}_4\text{Ru}_3\text{O}_{10}$ Structure: A10B3C4_oC68_64_2dfg_ad_2d-001

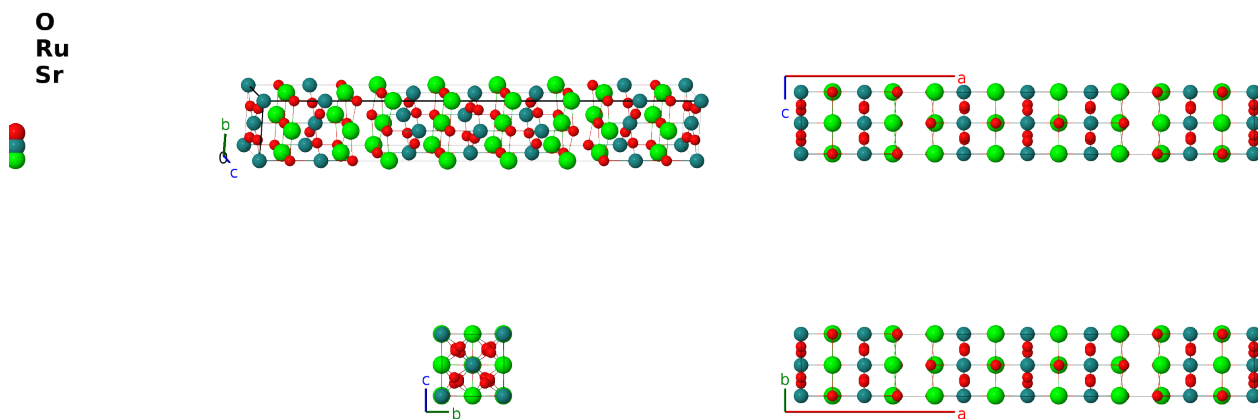
This structure previously used the label(s) **A10B3C4_oC68_64_2dfg_ad_2d**. Calls to these addresses will be redirected here.

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/XC67>

https://aflow.org/prototype-encyclopedia/A10B3C4_oC68_64_2dfg_ad_2d-001

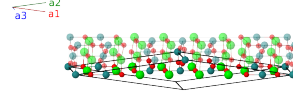


Prototype	$\text{O}_{10}\text{Ru}_3\text{Sr}_4$
AFLOW prototype label	A10B3C4_oC68_64_2dfg_ad_2d-001
ICSD	96729
CCDC	1656068
Pearson symbol	oC68
Space group number	64
Space group symbol	$Cmce$
AFLOW prototype command	<code>aflow --proto=A10B3C4_oC68_64_2dfg_ad_2d-001</code> <code>--params=a, b/a, c/a, x2, x3, x4, x5, x6, y7, z7, x8, y8, z8</code>

- (Crawford, 2002) placed $\text{Sr}_4\text{Ru}_3\text{O}_{10}$ in space group $Pbam$ #55, oP68, but found that it was very close to the current structure. Indeed, we derived this structure from the original structure by allowing a small amount of uncertainty in the atomic positions. In both cases the structure consists of triple-layer ruthenate separated by $2.37\text{\AA}$. In the original structure there are two of these layers in the primitive cell which are not equivalent. In the current structure there is only one triple-layer in the *primitive base-centered cell*, and so the layers in the *conventional cell* are equivalent.
- The lattice constants in the CIF for ICSD 96729 do not agree with the lattice constants in (Crawford, 2002), although the atomic positions are the same. We use the published lattice constants.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(4a)	Ru I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4a)	Ru I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}}$	(8d)	O I
$\mathbf{B}_4$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_5$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}}$	(8d)	O I
$\mathbf{B}_6$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}}$	(8d)	O II
$\mathbf{B}_8$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B}_9$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}}$	(8d)	O II
$\mathbf{B}_{10}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B}_{11}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}}$	(8d)	Ru II
$\mathbf{B}_{12}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	Ru II
$\mathbf{B}_{13}$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}}$	(8d)	Ru II
$\mathbf{B}_{14}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	Ru II
$\mathbf{B}_{15}$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2$	$=$	$ax_5 \hat{\mathbf{x}}$	(8d)	Sr I
$\mathbf{B}_{16}$	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	Sr I
$\mathbf{B}_{17}$	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2$	$=$	$-ax_5 \hat{\mathbf{x}}$	(8d)	Sr I
$\mathbf{B}_{18}$	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	Sr I
$\mathbf{B}_{19}$	$= x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2$	$=$	$ax_6 \hat{\mathbf{x}}$	(8d)	Sr II
$\mathbf{B}_{20}$	$= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a\left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	Sr II
$\mathbf{B}_{21}$	$= -x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2$	$=$	$-ax_6 \hat{\mathbf{x}}$	(8d)	Sr II
$\mathbf{B}_{22}$	$= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a\left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	Sr II
$\mathbf{B}_{23}$	$= -y_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_{24}$	$= \left(y_7 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_{25}$	$= -\left(y_7 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_{26}$	$= y_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_{27}$	$= (x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(16g)	O IV

$$\begin{aligned}
\mathbf{B}_{28} &= \begin{pmatrix} -x_8 + y_8 + \frac{1}{2} \\ x_8 + y_8 - \frac{1}{2} \\ z_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_8 + y_8 - \frac{1}{2} \\ -x_8 + y_8 + \frac{1}{2} \\ z_8 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_8 + y_8 - \frac{1}{2} \\ -x_8 + y_8 + \frac{1}{2} \\ z_8 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} & (16g) & \text{O IV} \\
\mathbf{B}_{29} &= \begin{pmatrix} -x_8 + y_8 - \frac{1}{2} \\ x_8 + y_8 + \frac{1}{2} \\ z_8 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_8 + y_8 + \frac{1}{2} \\ -x_8 + y_8 + \frac{1}{2} \\ z_8 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_8 + y_8 + \frac{1}{2} \\ -x_8 + y_8 + \frac{1}{2} \\ z_8 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}} & (16g) & \text{O IV} \\
\mathbf{B}_{30} &= \begin{pmatrix} x_8 + y_8 \\ x_8 - y_8 \\ z_8 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_8 - y_8 \\ x_8 + y_8 \\ z_8 \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_8 - y_8 \\ x_8 + y_8 \\ z_8 \end{pmatrix} \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (16g) & \text{O IV} \\
\mathbf{B}_{31} &= \begin{pmatrix} x_8 - y_8 \\ x_8 + y_8 \\ z_8 \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_8 + y_8 \\ x_8 - y_8 \\ z_8 \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_8 + y_8 \\ x_8 - y_8 \\ z_8 \end{pmatrix} \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (16g) & \text{O IV} \\
\mathbf{B}_{32} &= \begin{pmatrix} x_8 - y_8 + \frac{1}{2} \\ x_8 + y_8 + \frac{1}{2} \\ z_8 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_8 + y_8 + \frac{1}{2} \\ -x_8 + y_8 + \frac{1}{2} \\ z_8 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_8 + y_8 + \frac{1}{2} \\ -x_8 + y_8 + \frac{1}{2} \\ z_8 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}} & (16g) & \text{O IV} \\
\mathbf{B}_{33} &= \begin{pmatrix} x_8 + y_8 + \frac{1}{2} \\ x_8 - y_8 + \frac{1}{2} \\ z_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_8 - y_8 + \frac{1}{2} \\ x_8 + y_8 + \frac{1}{2} \\ z_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_8 - y_8 + \frac{1}{2} \\ x_8 + y_8 + \frac{1}{2} \\ z_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} & (16g) & \text{O IV} \\
\mathbf{B}_{34} &= \begin{pmatrix} x_8 + y_8 \\ x_8 - y_8 \\ z_8 \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_8 - y_8 \\ x_8 + y_8 \\ z_8 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_8 - y_8 \\ x_8 + y_8 \\ z_8 \end{pmatrix} \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (16g) & \text{O IV}
\end{aligned}$$

References

- [1] M. K. Crawford, R. L. Harlow, W. Marshall, Z. Li, G. Cao, R. L. Lindstrom, Q. Huang, and J. W. Lynn, *Structure and magnetism of single crystal $\text{Sr}_4\text{Ru}_3\text{O}_{10}$: A ferromagnetic triple-layer ruthenate*, Phys. Rev. B **65**, 214412 (2002), doi:10.1103/PhysRevB.65.214412.

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.