# Orthorhombic $Sr_4Ru_3O_{10}$ Structure: A10B3C4_oP68_55_2e2fgh2i_adef_2e2f-001

This structure previously used the label(s) `A10B3C4_oP68_55_2e2fgh2i_adef_2e2f`. Calls to these addresses will be redirected here.

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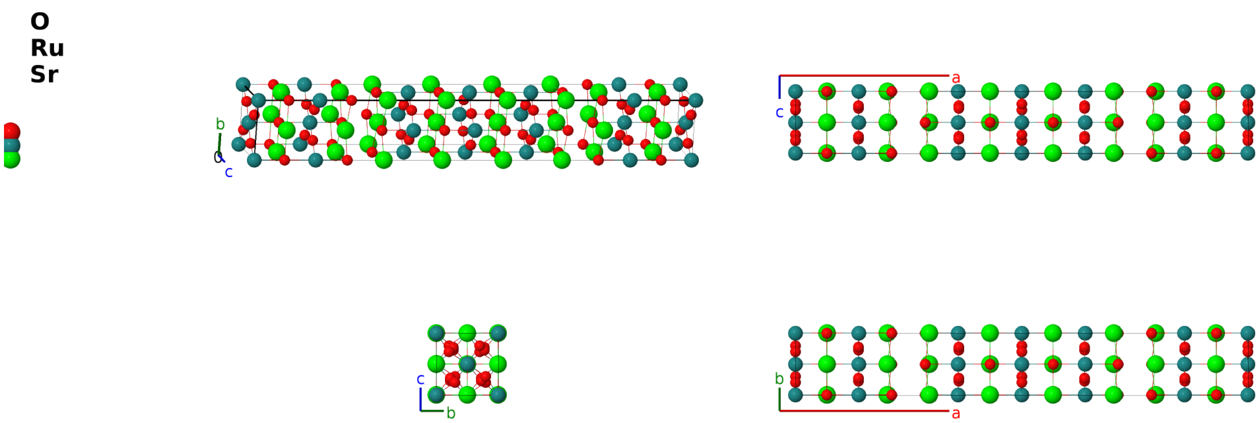
https://aflow.org/prototype-encyclopedia/PEKW

https://aflow.org/prototype-encyclopedia/A10B3C4_oP68_55_2e2fgh2i_adef_2e2f-001

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|---|---|
| **Prototype** | $O_{10}Ru_3Sr_4$ |
| **AFLOW prototype label** | A10B3C4_oP68_55_2e2fgh2i_adef_2e2f-001 |
| **ICSD** | 96729 |
| **CCDC** | 1656068 |
| **Pearson symbol** | oC68 |
| **Space group number** | 64 |
| **Space group symbol** | *Cmce* |
| **AFLOW prototype command** | `aflow --proto=A10B3C4_oP68_55_2e2fgh2i_adef_2e2f-001` `--params=`$a, b/a, c/a, x_2, x_3, x_4, x_5, x_6, y_7, z_7, x_8, y_8, z_8$ |

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- This structure consists of triple-layer ruthenate structures separated by 2.37Å from each other. In the *Pbam* #55 space group shown here there are two inequivalent stacks in the orthorhombic cell.
- This cell is very problematic. (Crawford, 2002) note that the x-ray scattering intensities are pseudo body-centered, but found that refining this structure in a body-centered cell with space group *Bbcm* (*Cmca* #64 in our standard orientation) led to non-positive definite thermal parameters. In that case there is only one triple-layer stack in the primitive cell, and the two stacks in the conventional orthorhombic cell are equivalent.

- If we use AFLOW with its default tolerance the structure also resolves into the smaller unit cell. The current cell can be recovered by using a smaller tolerance:

- aflow --proto=A10B3C4_oC68_64_2dfg_ad_2d:O:Ru:Sr --params=a,b/a,c/a,$x_2$,$z_3$,$z_4$,$z_5$,$z_6$,$z_7$,$z_8$,$z_9$,$z_{10}$,$z_{11}$,$z_{12}$,$x_{13}$,$y_{13}$,$x_{14}$,$y_{14}$,$x_{15}$,$y_{15}$,$z_{15}$,$x_{16}$,$y_{16}$,$z_{16}$ --tolerance=0.001 .

- Note that 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.

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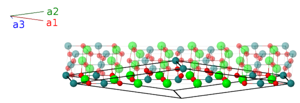
### Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$

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### 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 |
| $\mathbf{B_{28}}$ | = | $\left(-x_8+y_8+\frac{1}{2}\right)\mathbf{a}_1-\left(x_8+y_8-\frac{1}{2}\right)\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\mathbf{a}_3$ | = | $-a\left(x_8-\frac{1}{2}\right)\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\hat{\mathbf{z}}$ | (16g) | O IV |
| $\mathbf{B_{29}}$ | = | $-\left(x_8+y_8-\frac{1}{2}\right)\mathbf{a}_1+\left(-x_8+y_8+\frac{1}{2}\right)\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\mathbf{a}_3$ | = | $-a\left(x_8-\frac{1}{2}\right)\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\hat{\mathbf{z}}$ | (16g) | O IV |
| $\mathbf{B_{30}}$ | = | $(x_8+y_8)\,\mathbf{a}_1+(x_8-y_8)\,\mathbf{a}_2-z_8\,\mathbf{a}_3$ | = | $ax_8\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$ | (16g) | O IV |
| $\mathbf{B_{31}}$ | = | $-(x_8-y_8)\,\mathbf{a}_1-(x_8+y_8)\,\mathbf{a}_2-z_8\,\mathbf{a}_3$ | = | $-ax_8\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$ | (16g) | O IV |
| $\mathbf{B_{32}}$ | = | $\left(x_8-y_8+\frac{1}{2}\right)\mathbf{a}_1+\left(x_8+y_8+\frac{1}{2}\right)\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\mathbf{a}_3$ | = | $a\left(x_8+\frac{1}{2}\right)\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\hat{\mathbf{z}}$ | (16g) | O IV |
| $\mathbf{B_{33}}$ | = | $\left(x_8+y_8+\frac{1}{2}\right)\mathbf{a}_1+\left(x_8-y_8+\frac{1}{2}\right)\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\mathbf{a}_3$ | = | $a\left(x_8+\frac{1}{2}\right)\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\hat{\mathbf{z}}$ | (16g) | O IV |
| $\mathbf{B_{34}}$ | = | $-(x_8+y_8)\,\mathbf{a}_1-(x_8-y_8)\,\mathbf{a}_2+z_8\,\mathbf{a}_3$ | = | $-ax_8\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$ | (16g) | O IV |

## 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 $Sr_4Ru_3O_{10}$: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.