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

This structure originally had the label `A10B3C4_oP68_55_2e2fgh2i_adef_2e2f`. Calls to that address will be redirected here.

Cite this page as: 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.

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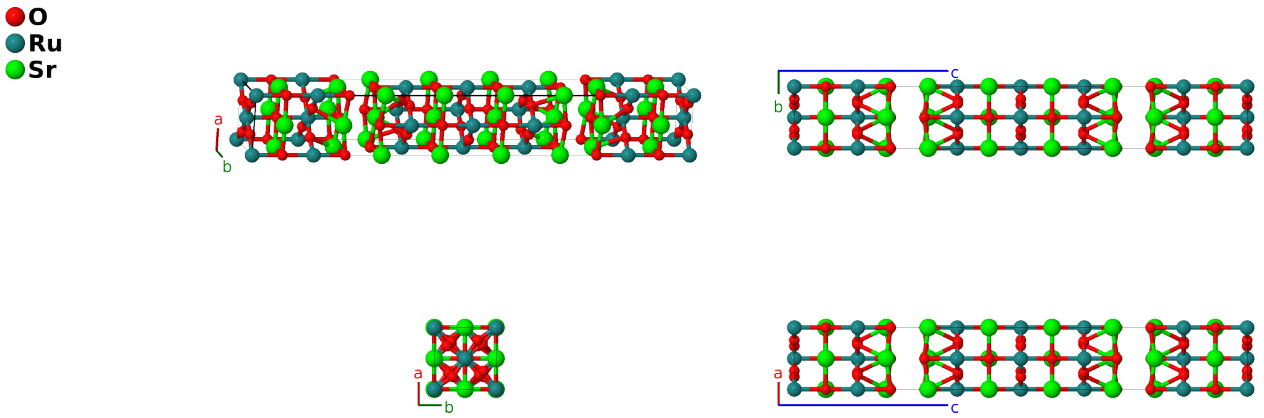
https://aflow.org/p/PEKW

https://aflow.org/p/A10B3C4_oP68_55_2e2fgh2i_adef_2e2f-001



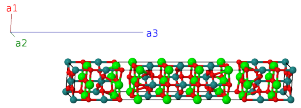
Prototype	$O_{10}Ru_3Sr_4$
AFLOW prototype label	A10B3C4_oP68_55_2e2fgh2i_adef_2e2f-001
ICSD	96729
Pearson symbol	oP68
Space group number	55
Space group symbol	*Pbam*
AFLOW prototype command	`aflow --proto=A10B3C4_oP68_55_2e2fgh2i_adef_2e2f-001 --params=`$a, b/a, c/a, z_3, z_4, z_5, z_6, z_7, z_8, z_9, z_{10}, z_{11}, z_{12}, x_{13}, y_{13}, x_{14}, y_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}$

- 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.

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ru I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(2a)	Ru I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	Ru II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	Ru II
$\mathbf{B_5}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_7}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_9}$	=	$z_4\,\mathbf{a}_3$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{11}}$	=	$-z_4\,\mathbf{a}_3$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{13}}$	=	$z_5\,\mathbf{a}_3$	=	$cz_5\,\hat{\mathbf{z}}$	(4e)	Ru III
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4e)	Ru III
$\mathbf{B_{15}}$	=	$-z_5\,\mathbf{a}_3$	=	$-cz_5\,\hat{\mathbf{z}}$	(4e)	Ru III
$\mathbf{B_{16}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4e)	Ru III
$\mathbf{B_{17}}$	=	$z_6\,\mathbf{a}_3$	=	$cz_6\,\hat{\mathbf{z}}$	(4e)	Sr I
$\mathbf{B_{18}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(4e)	Sr I
$\mathbf{B_{19}}$	=	$-z_6\,\mathbf{a}_3$	=	$-cz_6\,\hat{\mathbf{z}}$	(4e)	Sr I
$\mathbf{B_{20}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4e)	Sr I
$\mathbf{B_{21}}$	=	$z_7\,\mathbf{a}_3$	=	$cz_7\,\hat{\mathbf{z}}$	(4e)	Sr II
$\mathbf{B_{22}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(4e)	Sr II
$\mathbf{B_{23}}$	=	$-z_7\,\mathbf{a}_3$	=	$-cz_7\,\hat{\mathbf{z}}$	(4e)	Sr II
$\mathbf{B_{24}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4e)	Sr II
$\mathbf{B_{25}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4f)	O III
$\mathbf{B_{26}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_8\,\hat{\mathbf{z}}$	(4f)	O III
$\mathbf{B_{27}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(4f)	O III
$\mathbf{B_{28}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_8\,\hat{\mathbf{z}}$	(4f)	O III
$\mathbf{B_{29}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(4f)	O IV
$\mathbf{B_{30}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_9\,\hat{\mathbf{z}}$	(4f)	O IV
$\mathbf{B_{31}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(4f)	O IV

$\mathbf{B_{32}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_9\,\hat{\mathbf{z}}$	(4f)	O IV
$\mathbf{B_{33}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(4f)	Ru IV
$\mathbf{B_{34}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_{10}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_{10}\,\hat{\mathbf{z}}$	(4f)	Ru IV
$\mathbf{B_{35}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}}$	(4f)	Ru IV
$\mathbf{B_{36}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_{10}\,\hat{\mathbf{z}}$	(4f)	Ru IV
$\mathbf{B_{37}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(4f)	Sr III
$\mathbf{B_{38}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_{11}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_{11}\,\hat{\mathbf{z}}$	(4f)	Sr III
$\mathbf{B_{39}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}}$	(4f)	Sr III
$\mathbf{B_{40}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_{11}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_{11}\,\hat{\mathbf{z}}$	(4f)	Sr III
$\mathbf{B_{41}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(4f)	Sr IV
$\mathbf{B_{42}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_{12}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_{12}\,\hat{\mathbf{z}}$	(4f)	Sr IV
$\mathbf{B_{43}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} - cz_{12}\,\hat{\mathbf{z}}$	(4f)	Sr IV
$\mathbf{B_{44}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_{12}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_{12}\,\hat{\mathbf{z}}$	(4f)	Sr IV
$\mathbf{B_{45}}$	=	$x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2$	=	$ax_{13}\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}}$	(4g)	O V
$\mathbf{B_{46}}$	=	$-x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2$	=	$-ax_{13}\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}}$	(4g)	O V
$\mathbf{B_{47}}$	=	$-\left(x_{13} - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{13} + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_{13} - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_{13} + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	O V
$\mathbf{B_{48}}$	=	$\left(x_{13} + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{13} - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_{13} + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_{13} - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	O V
$\mathbf{B_{49}}$	=	$x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_{14}\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O VI
$\mathbf{B_{50}}$	=	$-x_{14}\,\mathbf{a}_1 - y_{14}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_{14}\,\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O VI
$\mathbf{B_{51}}$	=	$-\left(x_{14} - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{14} + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_{14} - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_{14} + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O VI
$\mathbf{B_{52}}$	=	$\left(x_{14} + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{14} - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_{14} + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_{14} - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O VI
$\mathbf{B_{53}}$	=	$x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3$	=	$ax_{15}\,\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}}$	(8i)	O VII
$\mathbf{B_{54}}$	=	$-x_{15}\,\mathbf{a}_1 - y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3$	=	$-ax_{15}\,\hat{\mathbf{x}} - by_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}}$	(8i)	O VII
$\mathbf{B_{55}}$	=	$-\left(x_{15} - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{15} + \frac{1}{2}\right)\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3$	=	$-a\left(x_{15} - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_{15} + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{15}\,\hat{\mathbf{z}}$	(8i)	O VII
$\mathbf{B_{56}}$	=	$\left(x_{15} + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{15} - \frac{1}{2}\right)\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3$	=	$a\left(x_{15} + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_{15} - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{15}\,\hat{\mathbf{z}}$	(8i)	O VII
$\mathbf{B_{57}}$	=	$-x_{15}\,\mathbf{a}_1 - y_{15}\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3$	=	$-ax_{15}\,\hat{\mathbf{x}} - by_{15}\,\hat{\mathbf{y}} - cz_{15}\,\hat{\mathbf{z}}$	(8i)	O VII
$\mathbf{B_{58}}$	=	$x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3$	=	$ax_{15}\,\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} - cz_{15}\,\hat{\mathbf{z}}$	(8i)	O VII
$\mathbf{B_{59}}$	=	$\left(x_{15} + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{15} - \frac{1}{2}\right)\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3$	=	$a\left(x_{15} + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_{15} - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}}$	(8i)	O VII
$\mathbf{B_{60}}$	=	$-\left(x_{15} - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{15} + \frac{1}{2}\right)\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3$	=	$-a\left(x_{15} - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_{15} + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}}$	(8i)	O VII
$\mathbf{B_{61}}$	=	$x_{16}\,\mathbf{a}_1 + y_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3$	=	$ax_{16}\,\hat{\mathbf{x}} + by_{16}\,\hat{\mathbf{y}} + cz_{16}\,\hat{\mathbf{z}}$	(8i)	O VIII
$\mathbf{B_{62}}$	=	$-x_{16}\,\mathbf{a}_1 - y_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3$	=	$-ax_{16}\,\hat{\mathbf{x}} - by_{16}\,\hat{\mathbf{y}} + cz_{16}\,\hat{\mathbf{z}}$	(8i)	O VIII
$\mathbf{B_{63}}$	=	$-\left(x_{16} - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{16} + \frac{1}{2}\right)\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3$	=	$-a\left(x_{16} - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_{16} + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{16}\,\hat{\mathbf{z}}$	(8i)	O VIII
$\mathbf{B_{64}}$	=	$\left(x_{16} + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{16} - \frac{1}{2}\right)\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3$	=	$a\left(x_{16} + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_{16} - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{16}\,\hat{\mathbf{z}}$	(8i)	O VIII
$\mathbf{B_{65}}$	=	$-x_{16}\,\mathbf{a}_1 - y_{16}\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3$	=	$-ax_{16}\,\hat{\mathbf{x}} - by_{16}\,\hat{\mathbf{y}} - cz_{16}\,\hat{\mathbf{z}}$	(8i)	O VIII
$\mathbf{B_{66}}$	=	$x_{16}\,\mathbf{a}_1 + y_{16}\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3$	=	$ax_{16}\,\hat{\mathbf{x}} + by_{16}\,\hat{\mathbf{y}} - cz_{16}\,\hat{\mathbf{z}}$	(8i)	O VIII

$$\mathbf{B_{67}} = \left(x_{16}+\tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_{16}-\tfrac{1}{2}\right)\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 = a\left(x_{16}+\tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{16}-\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{16}\,\hat{\mathbf{z}} \quad (8i) \quad \text{O VIII}$$

$$\mathbf{B_{68}} = -\left(x_{16}-\tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{16}+\tfrac{1}{2}\right)\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 = -a\left(x_{16}-\tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{16}+\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{16}\,\hat{\mathbf{z}} \quad (8i) \quad \text{O VIII}$$

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.