

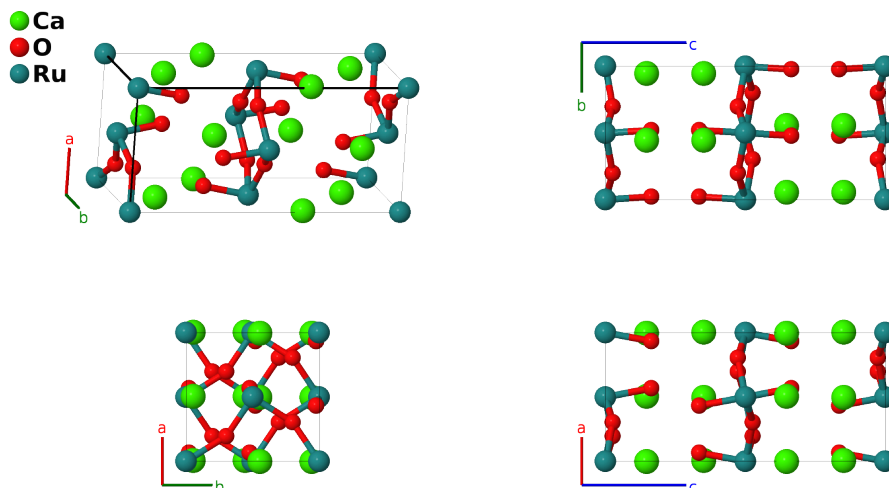
Ca₂RuO₄ Structure: A2B4C_oP28_61_c_2c_a-001

This structure originally had the label A2B4C_oP28_61_c_2c_a. 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.

<https://aflow.org/p/NDWA>

https://aflow.org/p/A2B4C_oP28_61_c_2c_a-001



Prototype	Ca ₂ O ₄ Ru
AFLOW prototype label	A2B4C_oP28_61_c_2c_a-001
ICSD	291033
Pearson symbol	oP28
Space group number	61
Space group symbol	<i>Pbca</i>
AFLOW prototype command	<code>aflow --proto=A2B4C_oP28_61_c_2c_a-001 --params=a, b/a, c/a, x₂, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄</code>

Other compounds with this structure

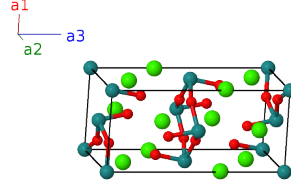
Ca_{2-x}Sr_xRuO₄, Nb₂UO₄

- (Friedt, 2001) never give the positions of the ruthenium atoms in this structure, however the composition of the crystal dictates that they can only be at the (4a) or (4b) Wyckoff positions, and the Ru-O distances given are consistent with the (4a) site.
- The authors identify a low temperature “S-*Pbca*” phase and a high temperature “L-*Pbca*” phase, with a phase transition in the range 350-400K. The major difference between the two phases is 4% elongation of the *c* axis in the L-*Pbca* phase, accompanied by a 4.5% contraction along the *b* axis, with the *a* axis being substantially unchanged. There is also a substantial change in the tilt of the oxygen octahedra surrounding the Ru atoms. Here we show the crystal in the S-*Pbca* phase using data taken at 180K.

- (Bertinshaw, 2019) identify S* and L* phases that have the same symmetry but stabilized by the application of an electric current.

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= 0$	$=$	0	(4a)	Ru I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4a)	Ru I
\mathbf{B}_3	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4a)	Ru I
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$	(4a)	Ru I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8c)	Ca I
\mathbf{B}_6	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Ca I
\mathbf{B}_7	$= -x_2 \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Ca I
\mathbf{B}_8	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8c)	Ca I
\mathbf{B}_9	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8c)	Ca I
\mathbf{B}_{10}	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + y_2 \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Ca I
\mathbf{B}_{11}	$= x_2 \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Ca I
\mathbf{B}_{12}	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8c)	Ca I
\mathbf{B}_{13}	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c)	O I
\mathbf{B}_{14}	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I
\mathbf{B}_{15}	$= -x_3 \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I
\mathbf{B}_{16}	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8c)	O I
\mathbf{B}_{17}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8c)	O I
\mathbf{B}_{18}	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I
\mathbf{B}_{19}	$= x_3 \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I
\mathbf{B}_{20}	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c)	O I
\mathbf{B}_{21}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8c)	O II
\mathbf{B}_{22}	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O II
\mathbf{B}_{23}	$= -x_4 \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O II

$$\begin{aligned}
\mathbf{B}_{24} &= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3 = a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (8c) & \text{O II} \\
\mathbf{B}_{25} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 = -ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (8c) & \text{O II} \\
\mathbf{B}_{26} &= (x_4 + \frac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3 = a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}} & (8c) & \text{O II} \\
\mathbf{B}_{27} &= x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3 = ax_4 \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}} & (8c) & \text{O II} \\
\mathbf{B}_{28} &= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3 = -a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (8c) & \text{O II}
\end{aligned}$$

References

- [1] O. Friedt, M. Braden, G. André, P. Adelman, S. Nakatsuji, and Y. Maeno, *Structural and magnetic aspects of the metal-insulator transition in $Ca_{2-x}Sr_xRuO_4$* , Phys. Rev. B **63**, 174432 (2001), doi:10.1103/PhysRevB.63.174432.

Found in

- [1] J. Bertinshaw, N. Gurung, P. Jorba, H. Liu, M. Schmid, D. Mantadakis, M. Daghofer, M. Krautloher, A. Jain, G. Ryu, O. Fabelo, P. Hansmann, G. Khaliullin, C. Pfleiderer, B. Keimer, and B. Kim, *Unique Crystal Structure of Ca_2RuO_4 in the Current Stabilized Semimetallic State*, Physical Review Letters **123**, 137204 (2019), doi:10.1103/PhysRevLett.123.137204.