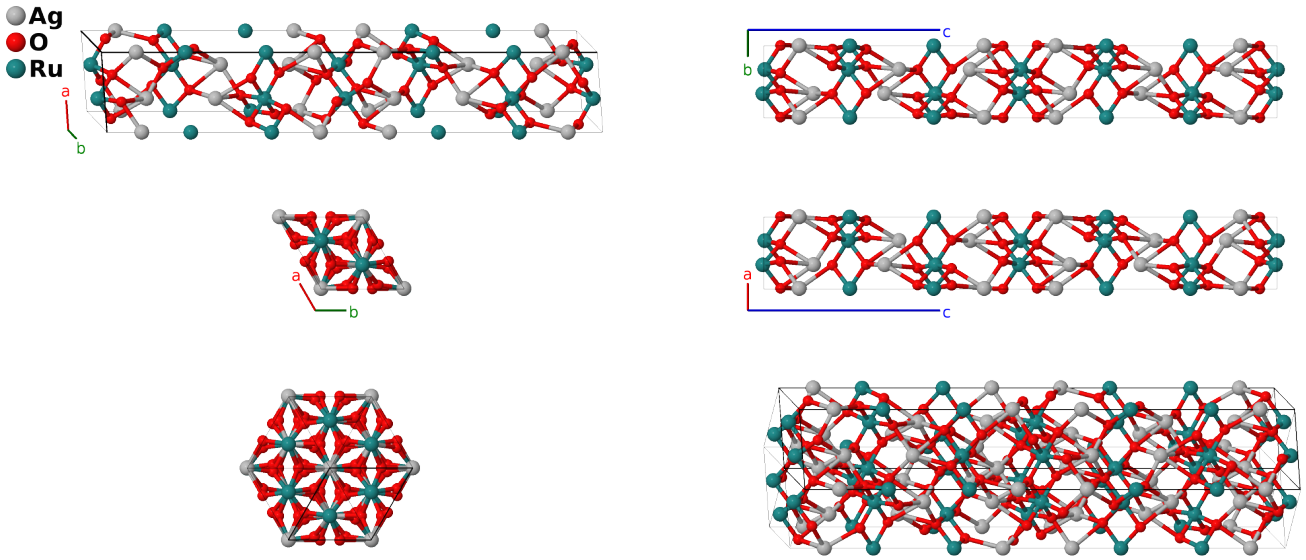
$AgRuO_3$ Structure: AB3C_hR20_167_c_f_c-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/QQE1

https://aflow.org/p/AB3C_hR20_167_c_f_c-001

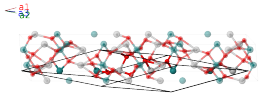


Prototype	AgO_3Ru
AFLOW prototype label	AB3C_hR20_167_c_f_c-001
ICSD	432362
Pearson symbol	hR20
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	`aflow --proto=AB3C_hR20_167_c_f_c-001 --params=`$a, c/a, x_1, x_2, x_3, y_3, z_3$

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(4c)	Ag I
$\mathbf{B_2}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1-\frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_1-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-c\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Ag I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-cx_1\,\hat{\mathbf{z}}$	(4c)	Ag I
$\mathbf{B_4}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_1+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Ag I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(4c)	Ru I
$\mathbf{B_6}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2-\frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-c\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Ru I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(4c)	Ru I
$\mathbf{B_8}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Ru I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_3-z_3\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_3-2y_3+z_3\right)\,\hat{\mathbf{y}} + \frac{1}{3}c\left(x_3+y_3+z_3\right)\,\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{10}}$	=	$z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(y_3-z_3\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_3-y_3-z_3\right)\,\hat{\mathbf{y}} + \frac{1}{3}c\left(x_3+y_3+z_3\right)\,\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{11}}$	=	$y_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_3-y_3\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_3+y_3-2z_3\right)\,\hat{\mathbf{y}} + \frac{1}{3}c\left(x_3+y_3+z_3\right)\,\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{12}}$	=	$-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_3-z_3\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(x_3-2y_3+z_3\right)\,\hat{\mathbf{y}} - \frac{1}{6}c\left(2x_3+2y_3+2z_3-3\right)\,\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{13}}$	=	$-\left(y_3-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3-\frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(y_3-z_3\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(2x_3-y_3-z_3\right)\,\hat{\mathbf{y}} - \frac{1}{6}c\left(2x_3+2y_3+2z_3-3\right)\,\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{14}}$	=	$-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(z_3-\frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_3-y_3\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(x_3+y_3-2z_3\right)\,\hat{\mathbf{y}} - \frac{1}{6}c\left(2x_3+2y_3+2z_3-3\right)\,\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{15}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_3-z_3\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(x_3-2y_3+z_3\right)\,\hat{\mathbf{y}} - \frac{1}{3}c\left(x_3+y_3+z_3\right)\,\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{16}}$	=	$-z_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(y_3-z_3\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(2x_3-y_3-z_3\right)\,\hat{\mathbf{y}} - \frac{1}{3}c\left(x_3+y_3+z_3\right)\,\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{17}}$	=	$-y_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_3-y_3\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(x_3+y_3-2z_3\right)\,\hat{\mathbf{y}} - \frac{1}{3}c\left(x_3+y_3+z_3\right)\,\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{18}}$	=	$\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_3-z_3\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_3-2y_3+z_3\right)\,\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_3+2y_3+2z_3+3\right)\,\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{19}}$	=	$\left(y_3+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(y_3-z_3\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_3-y_3-z_3\right)\,\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_3+2y_3+2z_3+3\right)\,\hat{\mathbf{z}}$	(12f)	O I
$\mathbf{B_{20}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_3-y_3\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_3+y_3-2z_3\right)\,\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_3+2y_3+2z_3+3\right)\,\hat{\mathbf{z}}$	(12f)	O I

References

[1] B. E. Prasad, S. Kanungo, M. Jansen, A. C. Komarek, B. Yan, P. Manuel, and C. Felser, *AgRuO$_3$, a Strongly Exchange-Coupled Honeycomb Compound Lacking Long-Range Magnetic Order*, Chem. Eur. J. **23**, 4680–4686 (2017), doi:10.1002/chem.201606057.

Found in

[1] W. Schnelle, B. E. Prasad, C. Felser, M. Jansen, E. V. Komleva, S. V. Streltsov, I. I. Mazin, D. Khalyavin, P. Manuel, S. Pal, D. V. S. Muthu, A. K. Sood, E. S. Klyushina, B. Lake, J.-C. Orain, and H. Luetkens, *Magnetic and electronic ordering phenomena in the Ru_2O_6-layer honeycomb lattice compound $AgRuO_3$*, Phys. Rev. B **103**, 214413 (2021), doi:10.1103/PhysRevB.103.214413.