$AgRuO_3$ Structure: AB3C_hR20_167_c_f_c-001

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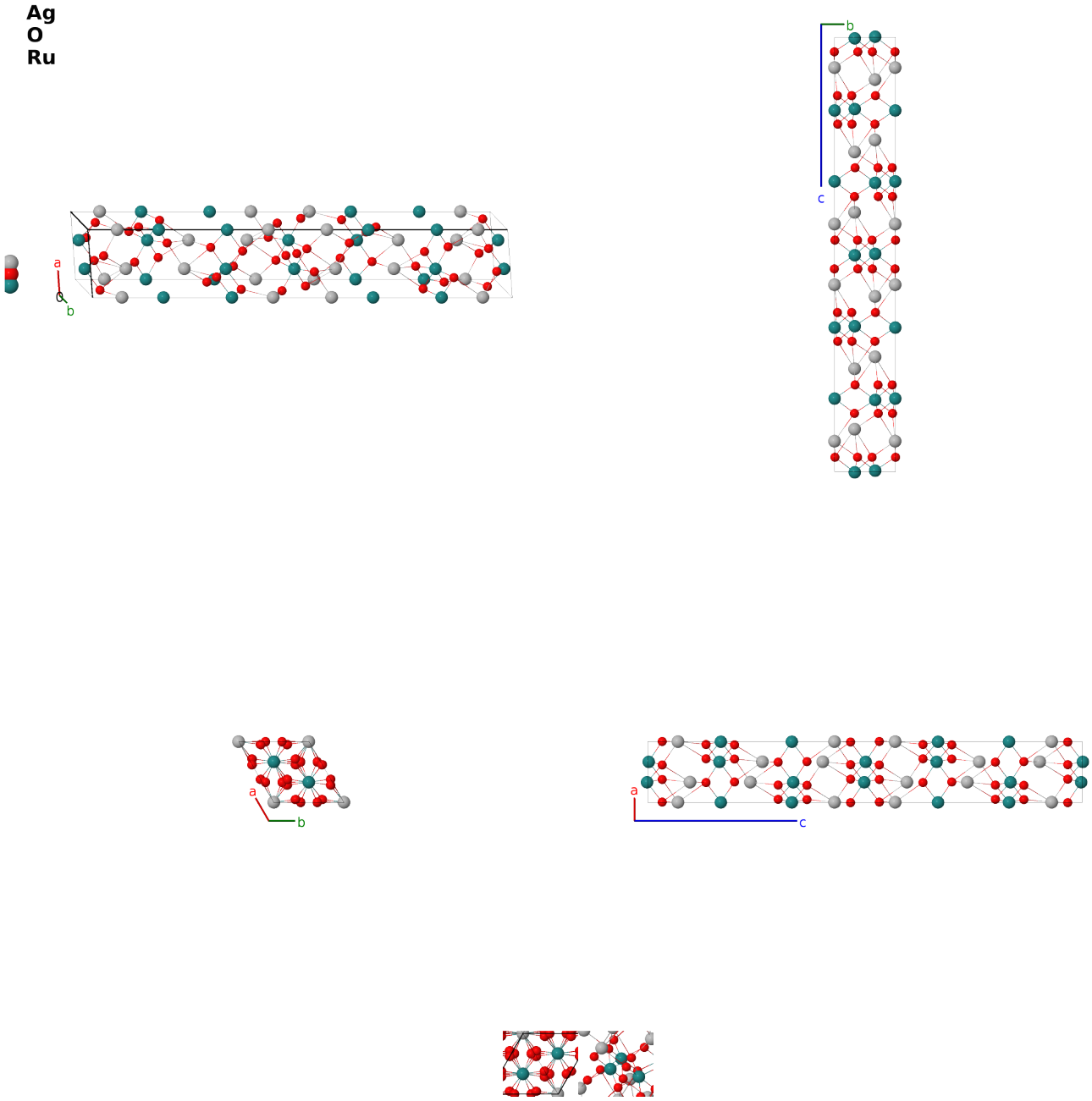
https://aflow.org/prototype-encyclopedia/QQE1

https://aflow.org/prototype-encyclopedia/AB3C_hR20_167_c_f_c-001



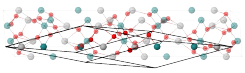
Prototype AgO_3Ru

AFLOW prototype label	AB3C_hR20_167_c_f_c-001
ICSD	432362
CCDC	1791377
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

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