

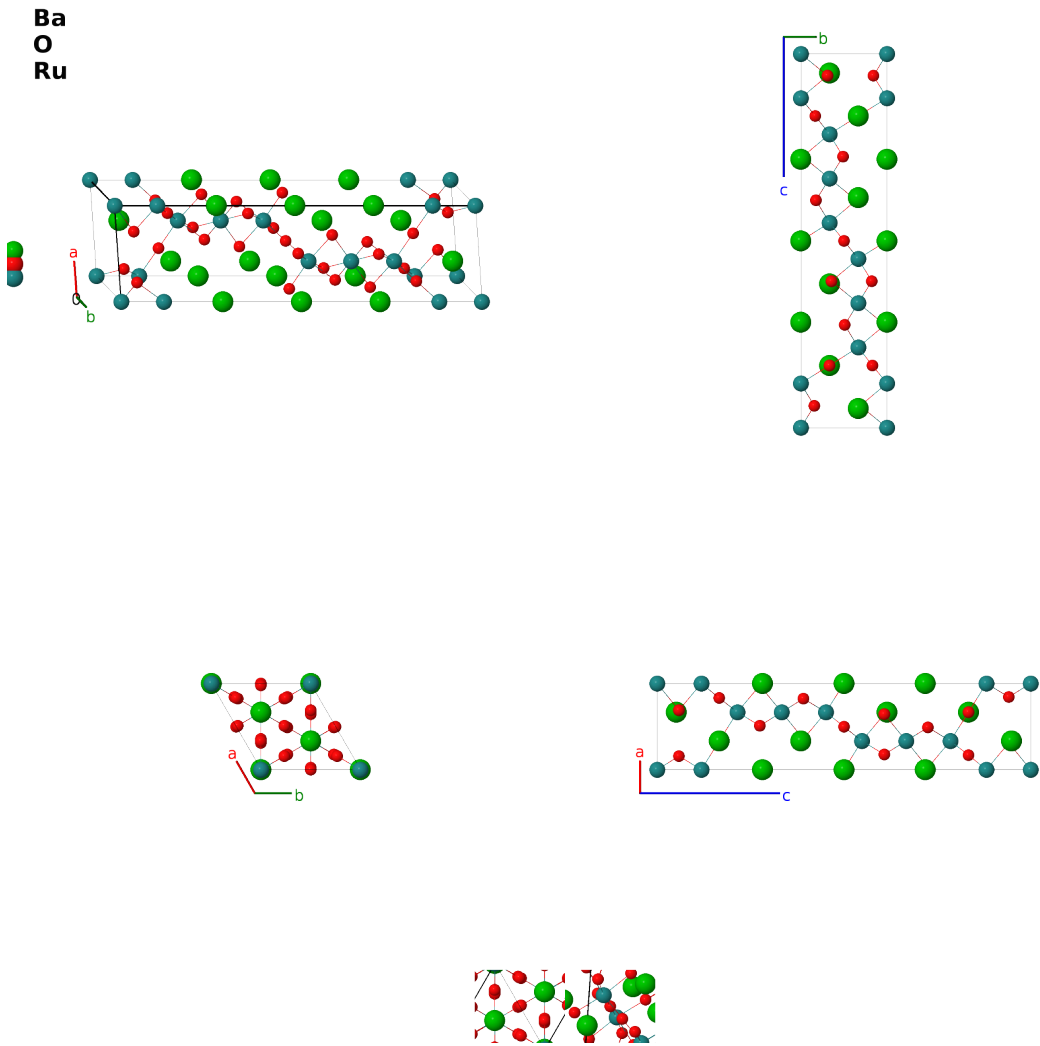
9R BaRuO₃ Structure: AB3C_hR15_166_bc_dh_ac-001

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<https://aflow.org/prototype-encyclopedia/ES6H>

https://aflow.org/prototype-encyclopedia/AB3C_hR15_166_bc_dh_ac-001



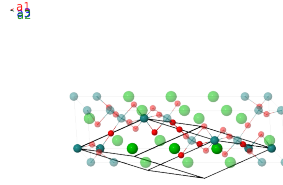
Prototype	BaO ₃ Ru
AFLOW prototype label	AB3C_hR15_166_bc_dh_ac-001
ICSD	10253
CCDC	1595108
Pearson symbol	hR15

Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=AB3C_hR15_166_bc_dh_ac-001</code> <code>--params=a, c/a, x₃, x₄, x₆, z₆</code>

- BaRuO₃ is found in four different phases distinguished by the stacking of the ruthenium atoms and their surrounding oxygens (Jin, 2008):
 - The ground state rhombohedral 9R structure (this page),
 - the hexagonal 4H BaMnO₃ structure,
 - the hexagonal 6H high-temperature BaTiO₃ structure, and
 - the cubic perovskite ($E2_1$) structure.
- (Jin, 2008) produced the three metastable states by heating the 9R phase to 1000° and subjecting it to pressures of 3 GPa, 5 GPa and 18 GPa, respectively.

Rhombohedral primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
 \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
 \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}
 \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(1a)	Ru I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(1b)	Ba I
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$cx_3 \hat{\mathbf{z}}$	(2c)	Ba II
$\mathbf{B}_4$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-cx_3 \hat{\mathbf{z}}$	(2c)	Ba II
$\mathbf{B}_5$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$cx_4 \hat{\mathbf{z}}$	(2c)	Ru II
$\mathbf{B}_6$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-cx_4 \hat{\mathbf{z}}$	(2c)	Ru II
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3d)	O I
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3d)	O I
$\mathbf{B}_9$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3d)	O I
$\mathbf{B}_{10}$	$= x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B}_{11}$	$= z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B}_{12}$	$= x_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h)	O II

$$\mathbf{B}_{13} = -z_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - x_6 \mathbf{a}_3 = \frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}} \quad (6h) \quad \text{O II}$$

$$\mathbf{B}_{14} = -x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 = -\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}} \quad (6h) \quad \text{O II}$$

$$\mathbf{B}_{15} = -x_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 - x_6 \mathbf{a}_3 = \frac{1}{\sqrt{3}}a(x_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}} \quad (6h) \quad \text{O II}$$

References

- [1] P. C. Donhoue, L. Katz, and R. Ward, *The Crystal Structure of Barium Ruthenium Oxide and Related Compounds*, Inorg. Chem. **4**, 306–310 (1965), doi:10.1021/ic50025a010.
- [2] C.-Q. Jin, J.-S. Zhou, J. B. Goodenough, Q. Q. Liu, J. G. Zhao, L. X. Yang, Y. Yu, R. C. Yu, T. Katsura, A. Shatskiy, and E. Ito, *High-pressure synthesis of the cubic perovskite BaRuO₃ and evolution of ferromagnetism in ARuO₃ (A = Ca, Sr, Ba) ruthenates*, Proc. Natl. Acad. Sci. **105**, 7115–7119 (2008), doi:10.1073/pnas.0710928105.

Found in

- [1] ICSD, Inorganic Crystal Structure Database. ID 23973.

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