

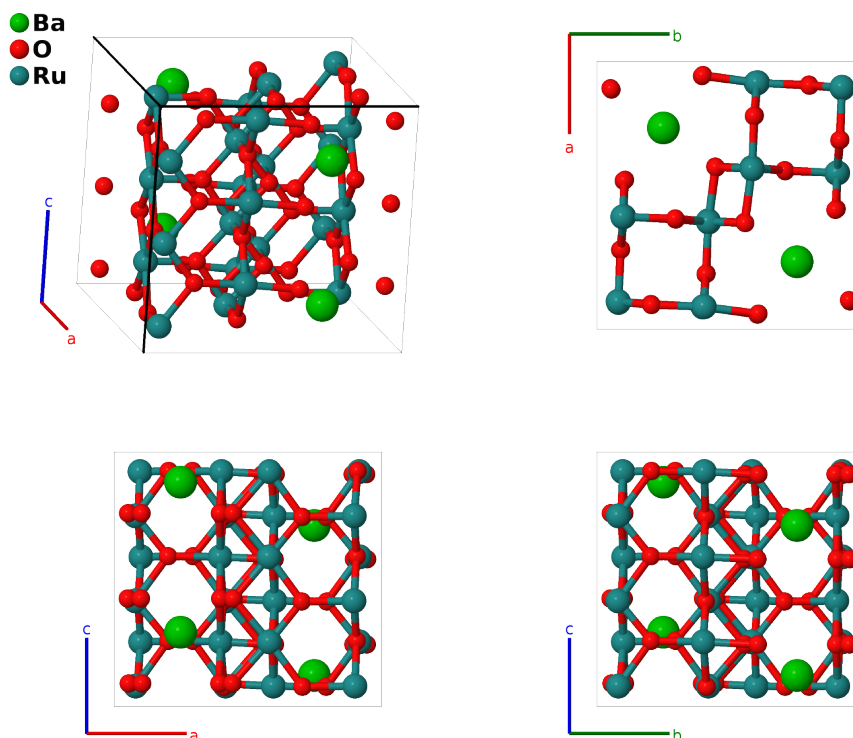
BaRu₆O₁₂ Structure:

AB12C6_tP76_85_2c_6g_3g-001

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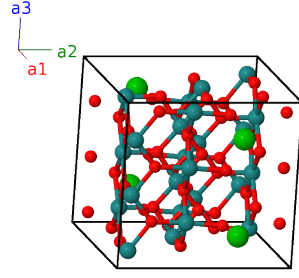
https://aflow.org/p/AB12C6_tP76_85_2c_6g_3g-001



Prototype	BaO ₁₂ Ru ₆
AFLOW prototype label	AB12C6_tP76_85_2c_6g_3g-001
ICSD	61387
Pearson symbol	tP76
Space group number	85
Space group symbol	$P4/n$
AFLOW prototype command	aflow --proto=AB12C6_tP76_85_2c_6g_3g-001 --params=a, c/a, z ₁ , z ₂ , x ₃ , y ₃ , z ₃ , x ₄ , y ₄ , z ₄ , x ₅ , y ₅ , z ₅ , x ₆ , y ₆ , z ₆ , x ₇ , y ₇ , z ₇ , x ₈ , y ₈ , z ₈ , x ₉ , y ₉ , z ₉ , x ₁₀ , y ₁₀ , z ₁₀ , x ₁₁ , y ₁₁ , z ₁₁

Simple Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2c)	Ba I
\mathbf{B}_2	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(2c)	Ba I
\mathbf{B}_3	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2c)	Ba II
\mathbf{B}_4	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(2c)	Ba II
\mathbf{B}_5	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_6	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_7	$= -\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_8	$= y_3 \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_9	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_{10}	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_{11}	$= \left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_{12}	$= -y_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{14}	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{15}	$= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{16}	$= y_4 \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{17}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{18}	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{19}	$= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{20}	$= -y_4 \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{21}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	O III
\mathbf{B}_{22}	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_5 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	O III
\mathbf{B}_{23}	$= -\left(y_5 - \frac{1}{2}\right) \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a\left(y_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	O III
\mathbf{B}_{24}	$= y_5 \mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	O III
\mathbf{B}_{25}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8g)	O III
\mathbf{B}_{26}	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8g)	O III
\mathbf{B}_{27}	$= \left(y_5 + \frac{1}{2}\right) \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a\left(y_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8g)	O III
\mathbf{B}_{28}	$= -y_5 \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8g)	O III

$$\begin{aligned}
\mathbf{B}_{66} &= \begin{pmatrix} (x_{10} + \frac{1}{2}) \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 - \\ z_{10} \mathbf{a}_3 \end{pmatrix} = a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} + a(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (8g) & \text{Ru II} \\
\mathbf{B}_{67} &= \begin{pmatrix} (y_{10} + \frac{1}{2}) \mathbf{a}_1 - x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 \end{pmatrix} = a(y_{10} + \frac{1}{2}) \hat{\mathbf{x}} - ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (8g) & \text{Ru II} \\
\mathbf{B}_{68} &= -y_{10} \mathbf{a}_1 + (x_{10} + \frac{1}{2}) \mathbf{a}_2 - z_{10} \mathbf{a}_3 = -ay_{10} \hat{\mathbf{x}} + a(x_{10} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (8g) & \text{Ru II} \\
\mathbf{B}_{69} &= \begin{pmatrix} x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 \end{pmatrix} = ax_{11} \hat{\mathbf{x}} + ay_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8g) & \text{Ru III} \\
\mathbf{B}_{70} &= -\begin{pmatrix} (x_{11} - \frac{1}{2}) \mathbf{a}_1 - (y_{11} - \frac{1}{2}) \mathbf{a}_2 + \\ z_{11} \mathbf{a}_3 \end{pmatrix} = -a(x_{11} - \frac{1}{2}) \hat{\mathbf{x}} - a(y_{11} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8g) & \text{Ru III} \\
\mathbf{B}_{71} &= -\begin{pmatrix} (y_{11} - \frac{1}{2}) \mathbf{a}_1 + x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 \end{pmatrix} = -a(y_{11} - \frac{1}{2}) \hat{\mathbf{x}} + ax_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8g) & \text{Ru III} \\
\mathbf{B}_{72} &= \begin{pmatrix} y_{11} \mathbf{a}_1 - (x_{11} - \frac{1}{2}) \mathbf{a}_2 + z_{11} \mathbf{a}_3 \end{pmatrix} = ay_{11} \hat{\mathbf{x}} - a(x_{11} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8g) & \text{Ru III} \\
\mathbf{B}_{73} &= \begin{pmatrix} -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 \end{pmatrix} = -ax_{11} \hat{\mathbf{x}} - ay_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (8g) & \text{Ru III} \\
\mathbf{B}_{74} &= \begin{pmatrix} (x_{11} + \frac{1}{2}) \mathbf{a}_1 + (y_{11} + \frac{1}{2}) \mathbf{a}_2 - \\ z_{11} \mathbf{a}_3 \end{pmatrix} = a(x_{11} + \frac{1}{2}) \hat{\mathbf{x}} + a(y_{11} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (8g) & \text{Ru III} \\
\mathbf{B}_{75} &= \begin{pmatrix} (y_{11} + \frac{1}{2}) \mathbf{a}_1 - x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 \end{pmatrix} = a(y_{11} + \frac{1}{2}) \hat{\mathbf{x}} - ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (8g) & \text{Ru III} \\
\mathbf{B}_{76} &= -y_{11} \mathbf{a}_1 + (x_{11} + \frac{1}{2}) \mathbf{a}_2 - z_{11} \mathbf{a}_3 = -ay_{11} \hat{\mathbf{x}} + a(x_{11} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (8g) & \text{Ru III}
\end{aligned}$$

References

- [1] C. C. Torardi, *Synthesis and crystal structure of BaRu₆O₁₂: An ordered stoichiometric hollandite*, Mater. Res. Bull. **20**, 705–713 (1985), doi:10.1016/0025-5408(85)90149-7.