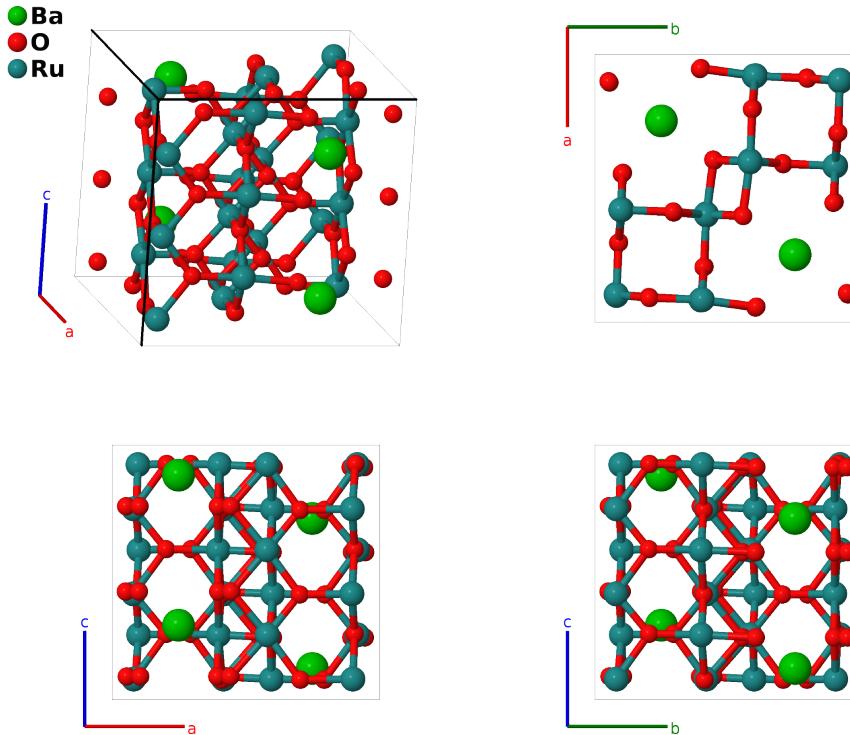


BaRu₆O₁₂ Structure: AB12C6_tP76_85_2c_6g_3g-001

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

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

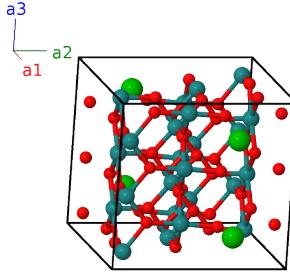
https://aflow.org/p/AB12C6_tP76_85_2c_6g_3g-001



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	<pre>aflow --proto=AB12C6_tP76_85_2c_6g_3g-001 --params=a, c/a, z1, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11</pre>

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	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_7	$-(y_3 - \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$-a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_8	$y_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$ay_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(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}	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_{11}	$(y_3 + \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_{12}	$-y_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$-ay_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(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}	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{15}	$-(y_4 - \frac{1}{2}) \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{16}	$y_4 \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$ay_4 \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(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}	$(x_4 + \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{19}	$(y_4 + \frac{1}{2}) \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{20}	$-y_4 \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$-ay_4 \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(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}	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	O III
\mathbf{B}_{23}	$-(y_5 - \frac{1}{2}) \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$-a(y_5 - \frac{1}{2}) \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8g)	O III
\mathbf{B}_{24}	$y_5 \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$ay_5 \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(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}	$(x_5 + \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8g)	O III
\mathbf{B}_{27}	$(y_5 + \frac{1}{2}) \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$a(y_5 + \frac{1}{2}) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8g)	O III
\mathbf{B}_{28}	$-y_5 \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$-ay_5 \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8g)	O III

\mathbf{B}_{29}	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8g)	O IV
\mathbf{B}_{30}	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8g)	O IV
\mathbf{B}_{31}	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8g)	O IV
\mathbf{B}_{32}	$y_6 \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8g)	O IV
\mathbf{B}_{33}	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8g)	O IV
\mathbf{B}_{34}	$(x_6 + \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8g)	O IV
\mathbf{B}_{35}	$(y_6 + \frac{1}{2}) \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$a(y_6 + \frac{1}{2}) \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8g)	O IV
\mathbf{B}_{36}	$-y_6 \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8g)	O IV
\mathbf{B}_{37}	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8g)	O V
\mathbf{B}_{38}	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8g)	O V
\mathbf{B}_{39}	$-(y_7 - \frac{1}{2}) \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-a(y_7 - \frac{1}{2}) \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8g)	O V
\mathbf{B}_{40}	$y_7 \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8g)	O V
\mathbf{B}_{41}	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8g)	O V
\mathbf{B}_{42}	$(x_7 + \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8g)	O V
\mathbf{B}_{43}	$(y_7 + \frac{1}{2}) \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$a(y_7 + \frac{1}{2}) \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8g)	O V
\mathbf{B}_{44}	$-y_7 \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8g)	O V
\mathbf{B}_{45}	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8g)	O VI
\mathbf{B}_{46}	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8g)	O VI
\mathbf{B}_{47}	$-(y_8 - \frac{1}{2}) \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-a(y_8 - \frac{1}{2}) \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8g)	O VI
\mathbf{B}_{48}	$y_8 \mathbf{a}_1 - (x_8 - \frac{1}{2}) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ay_8 \hat{\mathbf{x}} - a(x_8 - \frac{1}{2}) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8g)	O VI
\mathbf{B}_{49}	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8g)	O VI
\mathbf{B}_{50}	$(x_8 + \frac{1}{2}) \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8g)	O VI
\mathbf{B}_{51}	$(y_8 + \frac{1}{2}) \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$a(y_8 + \frac{1}{2}) \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8g)	O VI
\mathbf{B}_{52}	$-y_8 \mathbf{a}_1 + (x_8 + \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-ay_8 \hat{\mathbf{x}} + a(x_8 + \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8g)	O VI
\mathbf{B}_{53}	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8g)	Ru I
\mathbf{B}_{54}	$-(x_9 - \frac{1}{2}) \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_9 - \frac{1}{2}) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8g)	Ru I
\mathbf{B}_{55}	$-(y_9 - \frac{1}{2}) \mathbf{a}_1 + x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-a(y_9 - \frac{1}{2}) \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8g)	Ru I
\mathbf{B}_{56}	$y_9 \mathbf{a}_1 - (x_9 - \frac{1}{2}) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ay_9 \hat{\mathbf{x}} - a(x_9 - \frac{1}{2}) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8g)	Ru I
\mathbf{B}_{57}	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - ay_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8g)	Ru I
\mathbf{B}_{58}	$(x_9 + \frac{1}{2}) \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8g)	Ru I
\mathbf{B}_{59}	$(y_9 + \frac{1}{2}) \mathbf{a}_1 - x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$a(y_9 + \frac{1}{2}) \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8g)	Ru I
\mathbf{B}_{60}	$-y_9 \mathbf{a}_1 + (x_9 + \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-ay_9 \hat{\mathbf{x}} + a(x_9 + \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8g)	Ru I
\mathbf{B}_{61}	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + ay_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8g)	Ru II
\mathbf{B}_{62}	$-(x_{10} - \frac{1}{2}) \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} - a(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8g)	Ru II
\mathbf{B}_{63}	$-(y_{10} - \frac{1}{2}) \mathbf{a}_1 + x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$-a(y_{10} - \frac{1}{2}) \hat{\mathbf{x}} + ax_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8g)	Ru II
\mathbf{B}_{64}	$y_{10} \mathbf{a}_1 - (x_{10} - \frac{1}{2}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$ay_{10} \hat{\mathbf{x}} - a(x_{10} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8g)	Ru II
\mathbf{B}_{65}	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} - ay_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8g)	Ru II

B₆₆	$=$	$(x_{10} + \frac{1}{2}) \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} + a(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8g)	Ru II
B₆₇	$=$	$(y_{10} + \frac{1}{2}) \mathbf{a}_1 - x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$a(y_{10} + \frac{1}{2}) \hat{\mathbf{x}} - ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8g)	Ru II
B₆₈	$=$	$-y_{10} \mathbf{a}_1 + (x_{10} + \frac{1}{2}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-ay_{10} \hat{\mathbf{x}} + a(x_{10} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8g)	Ru II
B₆₉	$=$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}} + ay_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(8g)	Ru III
B₇₀	$=$	$-(x_{11} - \frac{1}{2}) \mathbf{a}_1 - (y_{11} - \frac{1}{2}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$-a(x_{11} - \frac{1}{2}) \hat{\mathbf{x}} - a(y_{11} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(8g)	Ru III
B₇₁	$=$	$-(y_{11} - \frac{1}{2}) \mathbf{a}_1 + x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$-a(y_{11} - \frac{1}{2}) \hat{\mathbf{x}} + ax_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(8g)	Ru III
B₇₂	$=$	$y_{11} \mathbf{a}_1 - (x_{11} - \frac{1}{2}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$ay_{11} \hat{\mathbf{x}} - a(x_{11} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(8g)	Ru III
B₇₃	$=$	$-x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{x}} - ay_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(8g)	Ru III
B₇₄	$=$	$(x_{11} + \frac{1}{2}) \mathbf{a}_1 + (y_{11} + \frac{1}{2}) \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$a(x_{11} + \frac{1}{2}) \hat{\mathbf{x}} + a(y_{11} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(8g)	Ru III
B₇₅	$=$	$(y_{11} + \frac{1}{2}) \mathbf{a}_1 - x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$a(y_{11} + \frac{1}{2}) \hat{\mathbf{x}} - ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(8g)	Ru III
B₇₆	$=$	$-y_{11} \mathbf{a}_1 + (x_{11} + \frac{1}{2}) \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-ay_{11} \hat{\mathbf{x}} + a(x_{11} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(8g)	Ru III

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.