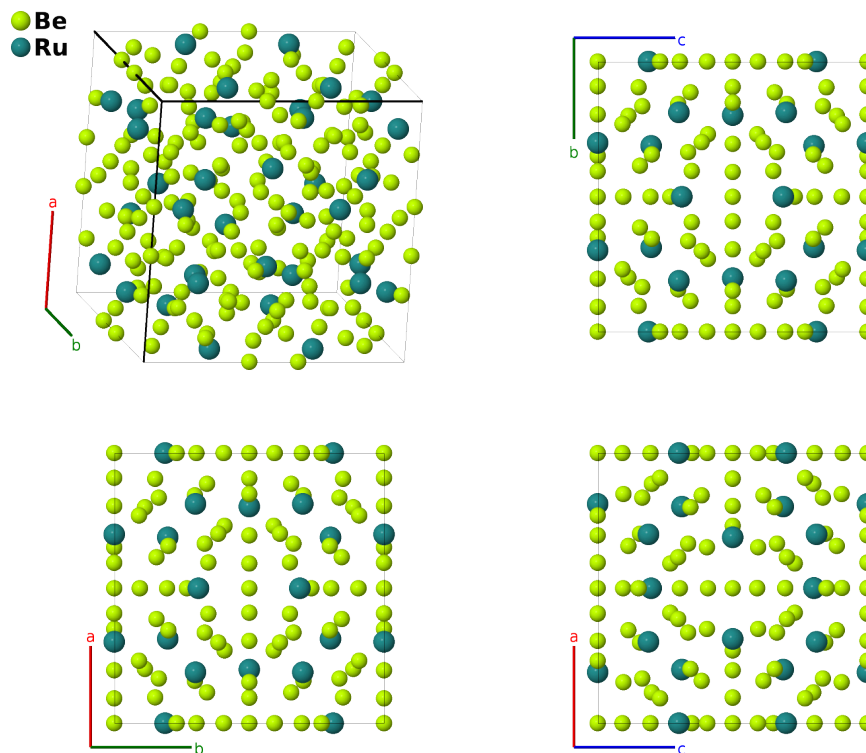


Ru₃Be₁₇ Structure: A17B3_cI160_204_def2gh_g-001

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/92TS>

https://aflow.org/p/A17B3_cI160_204_def2gh_g-001

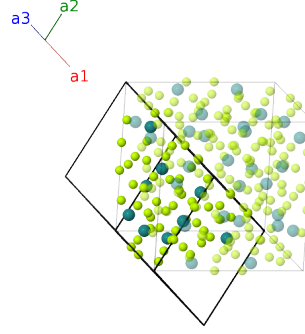


Prototype	Be ₁₇ Ru ₃
AFLOW prototype label	A17B3_cI160_204_def2gh_g-001
ICSD	58735
Pearson symbol	cI160
Space group number	204
Space group symbol	$Im\bar{3}$
AFLOW prototype command	aflow --proto=A17B3_cI160_204_def2gh_g-001 --params= <i>a, x₁, x₂, x₃, y₄, z₄, y₅, z₅, y₆, z₆, x₇, y₇, z₇</i>

Other compounds with this structure

Os₃Be₁₇

Body-centered Cubic primitive vectors



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

Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}}$	(12d)	Be I
\mathbf{B}_2	$= -x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}}$	(12d)	Be I
\mathbf{B}_3	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{y}}$	(12d)	Be I
\mathbf{B}_4	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{y}}$	(12d)	Be I
\mathbf{B}_5	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{z}}$	(12d)	Be I
\mathbf{B}_6	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{z}}$	(12d)	Be I
\mathbf{B}_7	$= \frac{1}{2} \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}}$	(12e)	Be II
\mathbf{B}_8	$= \frac{1}{2} \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}}$	(12e)	Be II
\mathbf{B}_9	$= x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(12e)	Be II
\mathbf{B}_{10}	$= -x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}}$	(12e)	Be II
\mathbf{B}_{11}	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(12e)	Be II
\mathbf{B}_{12}	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(12e)	Be II
\mathbf{B}_{13}	$= 2x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + 2x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16f)	Be III
\mathbf{B}_{14}	$= -2x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16f)	Be III
\mathbf{B}_{15}	$= -2x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16f)	Be III
\mathbf{B}_{16}	$= -2x_3 \mathbf{a}_1$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16f)	Be III
\mathbf{B}_{17}	$= -2x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 - 2x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16f)	Be III
\mathbf{B}_{18}	$= 2x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16f)	Be III
\mathbf{B}_{19}	$= 2x_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16f)	Be III
\mathbf{B}_{20}	$= 2x_3 \mathbf{a}_1$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16f)	Be III
\mathbf{B}_{21}	$= (y_4 + z_4) \mathbf{a}_1 + z_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}}$	(24g)	Be IV
\mathbf{B}_{22}	$= -(y_4 - z_4) \mathbf{a}_1 + z_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}}$	(24g)	Be IV
\mathbf{B}_{23}	$= (y_4 - z_4) \mathbf{a}_1 - z_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}}$	(24g)	Be IV
\mathbf{B}_{24}	$= -(y_4 + z_4) \mathbf{a}_1 - z_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}}$	(24g)	Be IV
\mathbf{B}_{25}	$= y_4 \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$az_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{z}}$	(24g)	Be IV
\mathbf{B}_{26}	$= -y_4 \mathbf{a}_1 - (y_4 - z_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$az_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{z}}$	(24g)	Be IV
\mathbf{B}_{27}	$= y_4 \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-az_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{z}}$	(24g)	Be IV
\mathbf{B}_{28}	$= -y_4 \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-az_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{z}}$	(24g)	Be IV
\mathbf{B}_{29}	$= z_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + (y_4 + z_4) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}}$	(24g)	Be IV
\mathbf{B}_{30}	$= z_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - (y_4 - z_4) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}}$	(24g)	Be IV

$$\begin{aligned}
\mathbf{B}_{66} &= -\frac{(x_7 - z_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 -}{(y_7 - z_7) \mathbf{a}_3} = -ay_7 \hat{\mathbf{x}} + az_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}} & (48h) & \text{Be VI} \\
\mathbf{B}_{67} &= -\frac{(x_7 + z_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 +}{(y_7 - z_7) \mathbf{a}_3} = ay_7 \hat{\mathbf{x}} - az_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}} & (48h) & \text{Be VI} \\
\mathbf{B}_{68} &= \frac{(x_7 - z_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 -}{(y_7 + z_7) \mathbf{a}_3} = -ay_7 \hat{\mathbf{x}} - az_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}} & (48h) & \text{Be VI} \\
\mathbf{B}_{69} &= -\frac{(y_7 + z_7) \mathbf{a}_1 - (x_7 + z_7) \mathbf{a}_2 -}{(x_7 + y_7) \mathbf{a}_3} = -ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} - az_7 \hat{\mathbf{z}} & (48h) & \text{Be VI} \\
\mathbf{B}_{70} &= \frac{(y_7 - z_7) \mathbf{a}_1 + (x_7 - z_7) \mathbf{a}_2 +}{(x_7 + y_7) \mathbf{a}_3} = ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} - az_7 \hat{\mathbf{z}} & (48h) & \text{Be VI} \\
\mathbf{B}_{71} &= -\frac{(y_7 - z_7) \mathbf{a}_1 + (x_7 + z_7) \mathbf{a}_2 +}{(x_7 - y_7) \mathbf{a}_3} = ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + az_7 \hat{\mathbf{z}} & (48h) & \text{Be VI} \\
\mathbf{B}_{72} &= \frac{(y_7 + z_7) \mathbf{a}_1 - (x_7 - z_7) \mathbf{a}_2 -}{(x_7 - y_7) \mathbf{a}_3} = -ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + az_7 \hat{\mathbf{z}} & (48h) & \text{Be VI} \\
\mathbf{B}_{73} &= -\frac{(x_7 + y_7) \mathbf{a}_1 - (y_7 + z_7) \mathbf{a}_2 -}{(x_7 + z_7) \mathbf{a}_3} = -az_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - ay_7 \hat{\mathbf{z}} & (48h) & \text{Be VI} \\
\mathbf{B}_{74} &= \frac{(x_7 + y_7) \mathbf{a}_1 + (y_7 - z_7) \mathbf{a}_2 +}{(x_7 - z_7) \mathbf{a}_3} = -az_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + ay_7 \hat{\mathbf{z}} & (48h) & \text{Be VI} \\
\mathbf{B}_{75} &= \frac{(x_7 - y_7) \mathbf{a}_1 - (y_7 - z_7) \mathbf{a}_2 +}{(x_7 + z_7) \mathbf{a}_3} = az_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - ay_7 \hat{\mathbf{z}} & (48h) & \text{Be VI} \\
\mathbf{B}_{76} &= -\frac{(x_7 - y_7) \mathbf{a}_1 + (y_7 + z_7) \mathbf{a}_2 -}{(x_7 - z_7) \mathbf{a}_3} = az_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + ay_7 \hat{\mathbf{z}} & (48h) & \text{Be VI} \\
\mathbf{B}_{77} &= -\frac{(x_7 + z_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 -}{(y_7 + z_7) \mathbf{a}_3} = -ay_7 \hat{\mathbf{x}} - az_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}} & (48h) & \text{Be VI} \\
\mathbf{B}_{78} &= \frac{(x_7 - z_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 +}{(y_7 - z_7) \mathbf{a}_3} = ay_7 \hat{\mathbf{x}} - az_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}} & (48h) & \text{Be VI} \\
\mathbf{B}_{79} &= \frac{(x_7 + z_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 -}{(y_7 - z_7) \mathbf{a}_3} = -ay_7 \hat{\mathbf{x}} + az_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}} & (48h) & \text{Be VI} \\
\mathbf{B}_{80} &= -\frac{(x_7 - z_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 +}{(y_7 + z_7) \mathbf{a}_3} = ay_7 \hat{\mathbf{x}} + az_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}} & (48h) & \text{Be VI}
\end{aligned}$$

References

- [1] D. E. Sands, Q. C. Johnson, O. H. Krikorian, and K. L. Kromholtz, *The Crystal Structure of Ru₃Be₁₇*, *Acta Cryst.* **15**, 1191–1195 (1962), doi:10.1107/S0567740871005028.

Found in

- [1] A. C. Larson and D. T. Cromer, *The Crystal Structure of YCd₆*, *Acta Crystallogr. Sect. B* **27**, 1875–1879 (1971), doi:10.1107/S0567740871005028.