

# Pu<sub>31</sub>Rh<sub>20</sub> Structure:

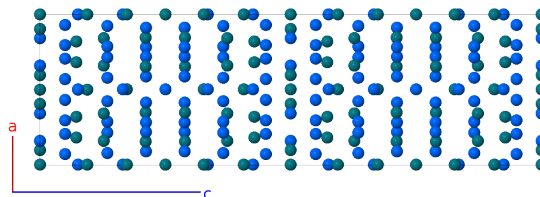
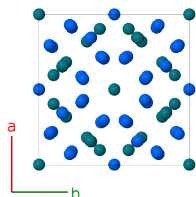
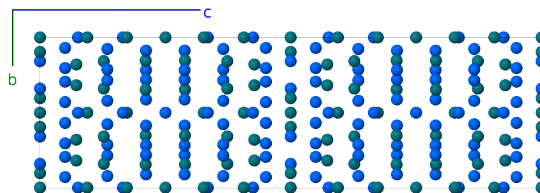
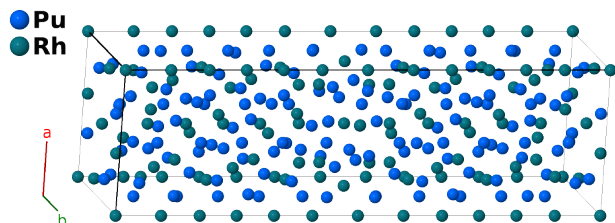
## A31B20\_tI204\_140\_b2gh3m\_ac2fh3l-001

This structure originally had the label A31B20\_tI204\_140\_b2gh3m\_ac2fh3l. Calls to that address will be redirected here.

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

[https://aflow.org/p/A31B20\\_tI204\\_140\\_b2gh3m\\_ac2fh3l-001](https://aflow.org/p/A31B20_tI204_140_b2gh3m_ac2fh3l-001)



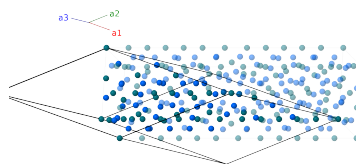
<b>Prototype</b>	Pu <sub>31</sub> Rh <sub>20</sub>
<b>AFLOW prototype label</b>	A31B20_tI204_140_b2gh3m_ac2fh3l-001
<b>ICSD</b>	1111
<b>Pearson symbol</b>	tI204
<b>Space group number</b>	140
<b>Space group symbol</b>	<i>I4/mcm</i>
<b>AFLOW prototype command</b>	aflow --proto=A31B20_tI204_140_b2gh3m_ac2fh3l-001 --params=a, c/a, z <sub>4</sub> , z <sub>5</sub> , z <sub>6</sub> , z <sub>7</sub> , x <sub>8</sub> , x <sub>9</sub> , x <sub>10</sub> , z <sub>10</sub> , x <sub>11</sub> , z <sub>11</sub> , x <sub>12</sub> , z <sub>12</sub> , x <sub>13</sub> , y <sub>13</sub> , z <sub>13</sub> , x <sub>14</sub> , y <sub>14</sub> , z <sub>14</sub> , x <sub>15</sub> , y <sub>15</sub> , z <sub>15</sub>

### Other compounds with this structure

Pu<sub>31</sub>Pt<sub>20</sub>, Ca<sub>31</sub>Sn<sub>20</sub>

### Body-centered Tetragonal primitive vectors

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



### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{1}{4} c \hat{\mathbf{z}}$	(4a)	Rh I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{3}{4} c \hat{\mathbf{z}}$	(4a)	Rh I
$\mathbf{B}_3$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4b)	Pu I
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4b)	Pu I
$\mathbf{B}_5$	$= 0$	$=$	$0$	(4c)	Rh II
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(4c)	Rh II
$\mathbf{B}_7$	$= z_4 \mathbf{a}_1 + z_4 \mathbf{a}_2$	$=$	$cz_4 \hat{\mathbf{z}}$	(8f)	Rh III
$\mathbf{B}_8$	$= -(z_4 - \frac{1}{2}) \mathbf{a}_1 - (z_4 - \frac{1}{2}) \mathbf{a}_2$	$=$	$-c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Rh III
$\mathbf{B}_9$	$= -z_4 \mathbf{a}_1 - z_4 \mathbf{a}_2$	$=$	$-cz_4 \hat{\mathbf{z}}$	(8f)	Rh III
$\mathbf{B}_{10}$	$= (z_4 + \frac{1}{2}) \mathbf{a}_1 + (z_4 + \frac{1}{2}) \mathbf{a}_2$	$=$	$c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Rh III
$\mathbf{B}_{11}$	$= z_5 \mathbf{a}_1 + z_5 \mathbf{a}_2$	$=$	$cz_5 \hat{\mathbf{z}}$	(8f)	Rh IV
$\mathbf{B}_{12}$	$= -(z_5 - \frac{1}{2}) \mathbf{a}_1 - (z_5 - \frac{1}{2}) \mathbf{a}_2$	$=$	$-c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Rh IV
$\mathbf{B}_{13}$	$= -z_5 \mathbf{a}_1 - z_5 \mathbf{a}_2$	$=$	$-cz_5 \hat{\mathbf{z}}$	(8f)	Rh IV
$\mathbf{B}_{14}$	$= (z_5 + \frac{1}{2}) \mathbf{a}_1 + (z_5 + \frac{1}{2}) \mathbf{a}_2$	$=$	$c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Rh IV
$\mathbf{B}_{15}$	$= (z_6 + \frac{1}{2}) \mathbf{a}_1 + z_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8g)	Pu II
$\mathbf{B}_{16}$	$= z_6 \mathbf{a}_1 + (z_6 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + cz_6 \hat{\mathbf{z}}$	(8g)	Pu II
$\mathbf{B}_{17}$	$= -z_6 \mathbf{a}_1 - (z_6 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_6 \hat{\mathbf{z}}$	(8g)	Pu II
$\mathbf{B}_{18}$	$= -(z_6 - \frac{1}{2}) \mathbf{a}_1 - z_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8g)	Pu II
$\mathbf{B}_{19}$	$= (z_7 + \frac{1}{2}) \mathbf{a}_1 + z_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8g)	Pu III
$\mathbf{B}_{20}$	$= z_7 \mathbf{a}_1 + (z_7 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + cz_7 \hat{\mathbf{z}}$	(8g)	Pu III
$\mathbf{B}_{21}$	$= -z_7 \mathbf{a}_1 - (z_7 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_7 \hat{\mathbf{z}}$	(8g)	Pu III
$\mathbf{B}_{22}$	$= -(z_7 - \frac{1}{2}) \mathbf{a}_1 - z_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8g)	Pu III
$\mathbf{B}_{23}$	$= (x_8 + \frac{1}{2}) \mathbf{a}_1 + x_8 \mathbf{a}_2 +$ $(2x_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + a(x_8 + \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	Pu IV
$\mathbf{B}_{24}$	$= -(x_8 - \frac{1}{2}) \mathbf{a}_1 - x_8 \mathbf{a}_2 -$ $(2x_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - a(x_8 - \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	Pu IV
$\mathbf{B}_{25}$	$= x_8 \mathbf{a}_1 - (x_8 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}}$	(8h)	Pu IV
$\mathbf{B}_{26}$	$= -x_8 \mathbf{a}_1 + (x_8 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}}$	(8h)	Pu IV
$\mathbf{B}_{27}$	$= (x_9 + \frac{1}{2}) \mathbf{a}_1 + x_9 \mathbf{a}_2 +$ $(2x_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + a(x_9 + \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	Rh V
$\mathbf{B}_{28}$	$= -(x_9 - \frac{1}{2}) \mathbf{a}_1 - x_9 \mathbf{a}_2 -$ $(2x_9 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - a(x_9 - \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	Rh V
$\mathbf{B}_{29}$	$= x_9 \mathbf{a}_1 - (x_9 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}}$	(8h)	Rh V
$\mathbf{B}_{30}$	$= -x_9 \mathbf{a}_1 + (x_9 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}}$	(8h)	Rh V
$\mathbf{B}_{31}$	$= (x_{10} + z_{10} + \frac{1}{2}) \mathbf{a}_1 +$ $(x_{10} + z_{10}) \mathbf{a}_2 + (2x_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + a(x_{10} + \frac{1}{2}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(16l)	Rh VI
$\mathbf{B}_{32}$	$= (-x_{10} + z_{10} + \frac{1}{2}) \mathbf{a}_1 -$ $(x_{10} - z_{10}) \mathbf{a}_2 - (2x_{10} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} - a(x_{10} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(16l)	Rh VI
$\mathbf{B}_{33}$	$= (x_{10} + z_{10}) \mathbf{a}_1 +$ $(-x_{10} + z_{10} + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} + ax_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(16l)	Rh VI



$$\begin{aligned}
\mathbf{B}_{57} &= \begin{pmatrix} (x_{13} + z_{13}) \mathbf{a}_1 - (y_{13} - z_{13}) \mathbf{a}_2 + \\ (x_{13} - y_{13}) \mathbf{a}_3 \end{pmatrix} = -ay_{13} \hat{\mathbf{x}} + ax_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (32m) & \text{Pu V} \\
\mathbf{B}_{58} &= \begin{pmatrix} -(x_{13} - z_{13}) \mathbf{a}_1 + \\ (y_{13} + z_{13}) \mathbf{a}_2 - (x_{13} - y_{13}) \mathbf{a}_3 \end{pmatrix} = ay_{13} \hat{\mathbf{x}} - ax_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (32m) & \text{Pu V} \\
\mathbf{B}_{59} &= \begin{pmatrix} (y_{13} - z_{13} + \frac{1}{2}) \mathbf{a}_1 - \\ (x_{13} + z_{13} - \frac{1}{2}) \mathbf{a}_2 - \\ (x_{13} - y_{13}) \mathbf{a}_3 \end{pmatrix} = -ax_{13} \hat{\mathbf{x}} + ay_{13} \hat{\mathbf{y}} - c(z_{13} - \frac{1}{2}) \hat{\mathbf{z}} & (32m) & \text{Pu V} \\
\mathbf{B}_{60} &= \begin{pmatrix} -(y_{13} + z_{13} - \frac{1}{2}) \mathbf{a}_1 + \\ (x_{13} - z_{13} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{13} - y_{13}) \mathbf{a}_3 \end{pmatrix} = ax_{13} \hat{\mathbf{x}} - ay_{13} \hat{\mathbf{y}} - c(z_{13} - \frac{1}{2}) \hat{\mathbf{z}} & (32m) & \text{Pu V} \\
\mathbf{B}_{61} &= \begin{pmatrix} (x_{13} - z_{13} + \frac{1}{2}) \mathbf{a}_1 + \\ (y_{13} - z_{13} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{13} + y_{13}) \mathbf{a}_3 \end{pmatrix} = ay_{13} \hat{\mathbf{x}} + ax_{13} \hat{\mathbf{y}} - c(z_{13} - \frac{1}{2}) \hat{\mathbf{z}} & (32m) & \text{Pu V} \\
\mathbf{B}_{62} &= \begin{pmatrix} -(x_{13} + z_{13} - \frac{1}{2}) \mathbf{a}_1 - \\ (y_{13} + z_{13} - \frac{1}{2}) \mathbf{a}_2 - \\ (x_{13} + y_{13}) \mathbf{a}_3 \end{pmatrix} = -ay_{13} \hat{\mathbf{x}} - ax_{13} \hat{\mathbf{y}} - c(z_{13} - \frac{1}{2}) \hat{\mathbf{z}} & (32m) & \text{Pu V} \\
\mathbf{B}_{63} &= \begin{pmatrix} -(y_{13} + z_{13}) \mathbf{a}_1 - \\ (x_{13} + z_{13}) \mathbf{a}_2 - (x_{13} + y_{13}) \mathbf{a}_3 \end{pmatrix} = -ax_{13} \hat{\mathbf{x}} - ay_{13} \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}} & (32m) & \text{Pu V} \\
\mathbf{B}_{64} &= \begin{pmatrix} (y_{13} - z_{13}) \mathbf{a}_1 + (x_{13} - z_{13}) \mathbf{a}_2 + \\ (x_{13} + y_{13}) \mathbf{a}_3 \end{pmatrix} = ax_{13} \hat{\mathbf{x}} + ay_{13} \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}} & (32m) & \text{Pu V} \\
\mathbf{B}_{65} &= \begin{pmatrix} -(x_{13} + z_{13}) \mathbf{a}_1 + \\ (y_{13} - z_{13}) \mathbf{a}_2 - (x_{13} - y_{13}) \mathbf{a}_3 \end{pmatrix} = ay_{13} \hat{\mathbf{x}} - ax_{13} \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}} & (32m) & \text{Pu V} \\
\mathbf{B}_{66} &= \begin{pmatrix} (x_{13} - z_{13}) \mathbf{a}_1 - (y_{13} + z_{13}) \mathbf{a}_2 + \\ (x_{13} - y_{13}) \mathbf{a}_3 \end{pmatrix} = -ay_{13} \hat{\mathbf{x}} + ax_{13} \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}} & (32m) & \text{Pu V} \\
\mathbf{B}_{67} &= \begin{pmatrix} (-y_{13} + z_{13} + \frac{1}{2}) \mathbf{a}_1 + \\ (x_{13} + z_{13} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{13} - y_{13}) \mathbf{a}_3 \end{pmatrix} = ax_{13} \hat{\mathbf{x}} - ay_{13} \hat{\mathbf{y}} + c(z_{13} + \frac{1}{2}) \hat{\mathbf{z}} & (32m) & \text{Pu V} \\
\mathbf{B}_{68} &= \begin{pmatrix} (y_{13} + z_{13} + \frac{1}{2}) \mathbf{a}_1 + \\ (-x_{13} + z_{13} + \frac{1}{2}) \mathbf{a}_2 - \\ (x_{13} - y_{13}) \mathbf{a}_3 \end{pmatrix} = -ax_{13} \hat{\mathbf{x}} + ay_{13} \hat{\mathbf{y}} + c(z_{13} + \frac{1}{2}) \hat{\mathbf{z}} & (32m) & \text{Pu V} \\
\mathbf{B}_{69} &= \begin{pmatrix} (-x_{13} + z_{13} + \frac{1}{2}) \mathbf{a}_1 + \\ (-y_{13} + z_{13} + \frac{1}{2}) \mathbf{a}_2 - \\ (x_{13} + y_{13}) \mathbf{a}_3 \end{pmatrix} = -ay_{13} \hat{\mathbf{x}} - ax_{13} \hat{\mathbf{y}} + c(z_{13} + \frac{1}{2}) \hat{\mathbf{z}} & (32m) & \text{Pu V} \\
\mathbf{B}_{70} &= \begin{pmatrix} (x_{13} + z_{13} + \frac{1}{2}) \mathbf{a}_1 + \\ (y_{13} + z_{13} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{13} + y_{13}) \mathbf{a}_3 \end{pmatrix} = ay_{13} \hat{\mathbf{x}} + ax_{13} \hat{\mathbf{y}} + c(z_{13} + \frac{1}{2}) \hat{\mathbf{z}} & (32m) & \text{Pu V} \\
\mathbf{B}_{71} &= \begin{pmatrix} (y_{14} + z_{14}) \mathbf{a}_1 + (x_{14} + z_{14}) \mathbf{a}_2 + \\ (x_{14} + y_{14}) \mathbf{a}_3 \end{pmatrix} = ax_{14} \hat{\mathbf{x}} + ay_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (32m) & \text{Pu VI} \\
\mathbf{B}_{72} &= \begin{pmatrix} -(y_{14} - z_{14}) \mathbf{a}_1 - \\ (x_{14} - z_{14}) \mathbf{a}_2 - (x_{14} + y_{14}) \mathbf{a}_3 \end{pmatrix} = -ax_{14} \hat{\mathbf{x}} - ay_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (32m) & \text{Pu VI} \\
\mathbf{B}_{73} &= \begin{pmatrix} (x_{14} + z_{14}) \mathbf{a}_1 - (y_{14} - z_{14}) \mathbf{a}_2 + \\ (x_{14} - y_{14}) \mathbf{a}_3 \end{pmatrix} = -ay_{14} \hat{\mathbf{x}} + ax_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (32m) & \text{Pu VI} \\
\mathbf{B}_{74} &= \begin{pmatrix} -(x_{14} - z_{14}) \mathbf{a}_1 + \\ (y_{14} + z_{14}) \mathbf{a}_2 - (x_{14} - y_{14}) \mathbf{a}_3 \end{pmatrix} = ay_{14} \hat{\mathbf{x}} - ax_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (32m) & \text{Pu VI} \\
\mathbf{B}_{75} &= \begin{pmatrix} (y_{14} - z_{14} + \frac{1}{2}) \mathbf{a}_1 - \\ (x_{14} + z_{14} - \frac{1}{2}) \mathbf{a}_2 - \\ (x_{14} - y_{14}) \mathbf{a}_3 \end{pmatrix} = -ax_{14} \hat{\mathbf{x}} + ay_{14} \hat{\mathbf{y}} - c(z_{14} - \frac{1}{2}) \hat{\mathbf{z}} & (32m) & \text{Pu VI}
\end{aligned}$$



$$\begin{aligned}
\mathbf{B}_{95} &= \begin{matrix} -(y_{15} + z_{15}) \mathbf{a}_1 - \\ (x_{15} + z_{15}) \mathbf{a}_2 - (x_{15} + y_{15}) \mathbf{a}_3 \end{matrix} = -ax_{15} \hat{\mathbf{x}} - ay_{15} \hat{\mathbf{y}} - cz_{15} \hat{\mathbf{z}} & (32m) & \text{Pu VII} \\
\mathbf{B}_{96} &= \begin{matrix} (y_{15} - z_{15}) \mathbf{a}_1 + (x_{15} - z_{15}) \mathbf{a}_2 + \\ (x_{15} + y_{15}) \mathbf{a}_3 \end{matrix} = ax_{15} \hat{\mathbf{x}} + ay_{15} \hat{\mathbf{y}} - cz_{15} \hat{\mathbf{z}} & (32m) & \text{Pu VII} \\
\mathbf{B}_{97} &= \begin{matrix} -(x_{15} + z_{15}) \mathbf{a}_1 + \\ (y_{15} - z_{15}) \mathbf{a}_2 - (x_{15} - y_{15}) \mathbf{a}_3 \end{matrix} = ay_{15} \hat{\mathbf{x}} - ax_{15} \hat{\mathbf{y}} - cz_{15} \hat{\mathbf{z}} & (32m) & \text{Pu VII} \\
\mathbf{B}_{98} &= \begin{matrix} (x_{15} - z_{15}) \mathbf{a}_1 - (y_{15} + z_{15}) \mathbf{a}_2 + \\ (x_{15} - y_{15}) \mathbf{a}_3 \end{matrix} = -ay_{15} \hat{\mathbf{x}} + ax_{15} \hat{\mathbf{y}} - cz_{15} \hat{\mathbf{z}} & (32m) & \text{Pu VII} \\
\mathbf{B}_{99} &= \begin{matrix} (-y_{15} + z_{15} + \frac{1}{2}) \mathbf{a}_1 + \\ (x_{15} + z_{15} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{15} - y_{15}) \mathbf{a}_3 \end{matrix} = ax_{15} \hat{\mathbf{x}} - ay_{15} \hat{\mathbf{y}} + c(z_{15} + \frac{1}{2}) \hat{\mathbf{z}} & (32m) & \text{Pu VII} \\
\mathbf{B}_{100} &= \begin{matrix} (y_{15} + z_{15} + \frac{1}{2}) \mathbf{a}_1 + \\ (-x_{15} + z_{15} + \frac{1}{2}) \mathbf{a}_2 - \\ (x_{15} - y_{15}) \mathbf{a}_3 \end{matrix} = -ax_{15} \hat{\mathbf{x}} + ay_{15} \hat{\mathbf{y}} + c(z_{15} + \frac{1}{2}) \hat{\mathbf{z}} & (32m) & \text{Pu VII} \\
\mathbf{B}_{101} &= \begin{matrix} (-x_{15} + z_{15} + \frac{1}{2}) \mathbf{a}_1 + \\ (-y_{15} + z_{15} + \frac{1}{2}) \mathbf{a}_2 - \\ (x_{15} + y_{15}) \mathbf{a}_3 \end{matrix} = -ay_{15} \hat{\mathbf{x}} - ax_{15} \hat{\mathbf{y}} + c(z_{15} + \frac{1}{2}) \hat{\mathbf{z}} & (32m) & \text{Pu VII} \\
\mathbf{B}_{102} &= \begin{matrix} (x_{15} + z_{15} + \frac{1}{2}) \mathbf{a}_1 + \\ (y_{15} + z_{15} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{15} + y_{15}) \mathbf{a}_3 \end{matrix} = ay_{15} \hat{\mathbf{x}} + ax_{15} \hat{\mathbf{y}} + c(z_{15} + \frac{1}{2}) \hat{\mathbf{z}} & (32m) & \text{Pu VII}
\end{aligned}$$

## References

- [1] D. T. Cromer and A. C. Larson, *The Crystal Structure of Pu<sub>31</sub>Pt<sub>20</sub> and Pu<sub>31</sub>Rh<sub>20</sub>*, Acta Crystallogr. Sect. B **33**, 2620–2627 (1977), doi:10.1107/S0567740877009030.