

# Ru<sub>11</sub>B<sub>8</sub> Structure: A8B11\_oP38\_55\_3gh\_b2g3h-001

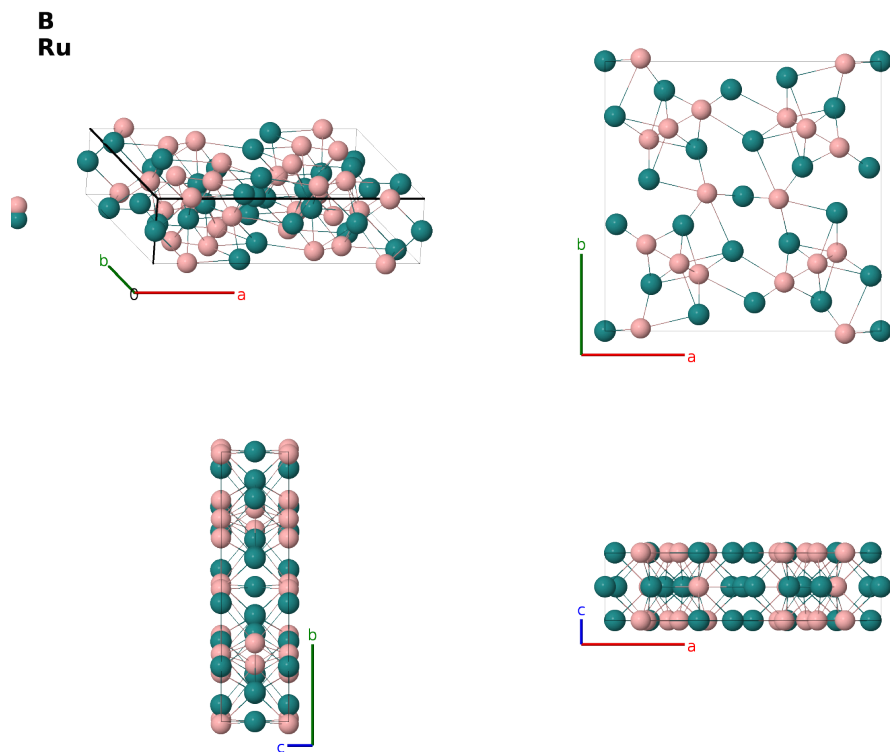
This structure previously used the label(s) **A8B11\_oP38\_55\_3gh\_a3g2h**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/6FNW>

[https://aflow.org/prototype-encyclopedia/A8B11\\_oP38\\_55\\_3gh\\_b2g3h-001](https://aflow.org/prototype-encyclopedia/A8B11_oP38_55_3gh_b2g3h-001)



|                         |                                                                                                                                                                                                                                                                                                                                                                             |
|-------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype               | B <sub>8</sub> Ru <sub>11</sub>                                                                                                                                                                                                                                                                                                                                             |
| AFLOW prototype label   | A8B11_oP38_55_3gh_b2g3h-001                                                                                                                                                                                                                                                                                                                                                 |
| ICSD                    | 43663                                                                                                                                                                                                                                                                                                                                                                       |
| CCDC                    | 1613136                                                                                                                                                                                                                                                                                                                                                                     |
| Pearson symbol          | oP38                                                                                                                                                                                                                                                                                                                                                                        |
| Space group number      | 55                                                                                                                                                                                                                                                                                                                                                                          |
| Space group symbol      | <i>Pbam</i>                                                                                                                                                                                                                                                                                                                                                                 |
| AFLOW prototype command | <code>aflow --proto=A8B11_oP38_55_3gh_b2g3h-001</code><br><code>--params=a, b/a, c/a, x<sub>2</sub>, y<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, x<sub>7</sub>, y<sub>7</sub>, x<sub>8</sub>, y<sub>8</sub>, x<sub>9</sub>, y<sub>9</sub>, x<sub>10</sub>, y<sub>10</sub></code> |

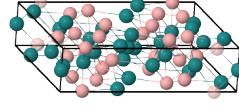
## Simple Orthorhombic primitive vectors

a<sub>2</sub>a<sub>3</sub>  
a<sub>1</sub>

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



## Basis vectors

|                   | Lattice<br>coordinates                                                                              |     | Cartesian<br>coordinates                                                                                          | Wyckoff<br>position | Atom<br>type |
|-------------------|-----------------------------------------------------------------------------------------------------|-----|-------------------------------------------------------------------------------------------------------------------|---------------------|--------------|
| $\mathbf{B}_1$    | $= \frac{1}{2} \mathbf{a}_3$                                                                        | $=$ | $\frac{1}{2} c \hat{\mathbf{z}}$                                                                                  | (2b)                | Ru I         |
| $\mathbf{B}_2$    | $= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$                  | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$                | (2b)                | Ru I         |
| $\mathbf{B}_3$    | $= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$                                                             | $=$ | $ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}}$                                                                   | (4g)                | B I          |
| $\mathbf{B}_4$    | $= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$                                                            | $=$ | $-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}}$                                                                  | (4g)                | B I          |
| $\mathbf{B}_5$    | $= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2$                            | $=$ | $-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}}$                                  | (4g)                | B I          |
| $\mathbf{B}_6$    | $= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2$                             | $=$ | $a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}}$                                   | (4g)                | B I          |
| $\mathbf{B}_7$    | $= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$                                                             | $=$ | $ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}}$                                                                   | (4g)                | B II         |
| $\mathbf{B}_8$    | $= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$                                                            | $=$ | $-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}}$                                                                  | (4g)                | B II         |
| $\mathbf{B}_9$    | $= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2$                            | $=$ | $-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}}$                                  | (4g)                | B II         |
| $\mathbf{B}_{10}$ | $= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2$                             | $=$ | $a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}}$                                   | (4g)                | B II         |
| $\mathbf{B}_{11}$ | $= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$                                                             | $=$ | $ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}}$                                                                   | (4g)                | B III        |
| $\mathbf{B}_{12}$ | $= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$                                                            | $=$ | $-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}}$                                                                  | (4g)                | B III        |
| $\mathbf{B}_{13}$ | $= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2$                            | $=$ | $-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}}$                                  | (4g)                | B III        |
| $\mathbf{B}_{14}$ | $= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2$                             | $=$ | $a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}}$                                   | (4g)                | B III        |
| $\mathbf{B}_{15}$ | $= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$                                                             | $=$ | $ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}}$                                                                   | (4g)                | Ru II        |
| $\mathbf{B}_{16}$ | $= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$                                                            | $=$ | $-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}}$                                                                  | (4g)                | Ru II        |
| $\mathbf{B}_{17}$ | $= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2$                            | $=$ | $-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}}$                                  | (4g)                | Ru II        |
| $\mathbf{B}_{18}$ | $= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2$                             | $=$ | $a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}}$                                   | (4g)                | Ru II        |
| $\mathbf{B}_{19}$ | $= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2$                                                             | $=$ | $ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}}$                                                                   | (4g)                | Ru III       |
| $\mathbf{B}_{20}$ | $= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2$                                                            | $=$ | $-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}}$                                                                  | (4g)                | Ru III       |
| $\mathbf{B}_{21}$ | $= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2$                            | $=$ | $-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}}$                                  | (4g)                | Ru III       |
| $\mathbf{B}_{22}$ | $= (x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2$                             | $=$ | $a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}}$                                   | (4g)                | Ru III       |
| $\mathbf{B}_{23}$ | $= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$                                  | $=$ | $ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$                                  | (4h)                | B IV         |
| $\mathbf{B}_{24}$ | $= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$                                 | $=$ | $-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$                                 | (4h)                | B IV         |
| $\mathbf{B}_{25}$ | $= -(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$ | $=$ | $-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$ | (4h)                | B IV         |
| $\mathbf{B}_{26}$ | $= (x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$  | $=$ | $a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$  | (4h)                | B IV         |
| $\mathbf{B}_{27}$ | $= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$                                  | $=$ | $ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$                                  | (4h)                | Ru IV        |

$$\begin{aligned}
\mathbf{B}_{28} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Ru IV} \\
\mathbf{B}_{29} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Ru IV} \\
\mathbf{B}_{30} &= \left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_8 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Ru IV} \\
\mathbf{B}_{31} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Ru V} \\
\mathbf{B}_{32} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Ru V} \\
\mathbf{B}_{33} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Ru V} \\
\mathbf{B}_{34} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Ru V} \\
\mathbf{B}_{35} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Ru VI} \\
\mathbf{B}_{36} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Ru VI} \\
\mathbf{B}_{37} &= -\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -a\left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Ru VI} \\
\mathbf{B}_{38} &= \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= a\left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} &(4h) &\text{Ru VI}
\end{aligned}$$

## References

[1] J. Åselius, *The Crystal Structure of Ru<sub>11</sub>B<sub>8</sub>*, Acta Chem. Scand. **14**, 2169–2176 (1960), doi:10.3891/acta.chem.scand.14-2169.

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