$Ru_{11}B_8$ Structure: A8B11_oP38_55_3gh_b2g3h-001

This structure originally had the label `A8B11_oP38_55_g3h_a3g2h`. Calls to that address will be redirected here.

https://aflow.org/p/6FNW

https://aflow.org/p/A8B11_oP38_55_3gh_b2g3h-001
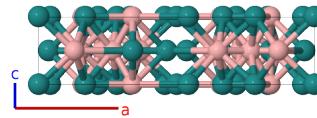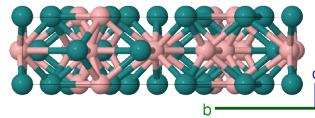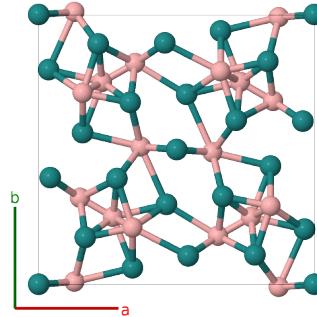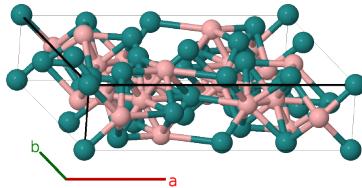
Prototype	B_8Ru_{11}
AFLOW prototype label	A8B11_oP38_55_3gh_b2g3h-001
ICSD	43663
Pearson symbol	oP38
Space group number	55
Space group symbol	$Pbam$
AFLOW prototype command	aflow --proto=A8B11_oP38_55_3gh_b2g3h-001 --params=$a, b/a, c/a, x_2, y_2, x_3, y_3, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7, x_8, y_8, x_9, y_9, x_{10}, y_{10}$

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$

$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
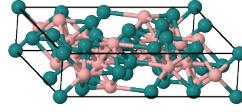
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom 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
$\mathbf{B_5}$	$=$	$-\left(x_2 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_2 + \frac{1}{2}\right)\mathbf{a_2}$	$=$	$-a\left(x_2 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}}$	(4g)	B I
$\mathbf{B_6}$	$=$	$\left(x_2 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_2 - \frac{1}{2}\right)\mathbf{a_2}$	$=$	$a\left(x_2 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\hat{\mathbf{y}}$	(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
$\mathbf{B_9}$	$=$	$-\left(x_3 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_3 + \frac{1}{2}\right)\mathbf{a_2}$	$=$	$-a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}}$	(4g)	B II
$\mathbf{B_{10}}$	$=$	$\left(x_3 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_3 - \frac{1}{2}\right)\mathbf{a_2}$	$=$	$a\left(x_3 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}}$	(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
$\mathbf{B_{13}}$	$=$	$-\left(x_4 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_4 + \frac{1}{2}\right)\mathbf{a_2}$	$=$	$-a\left(x_4 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}}$	(4g)	B III
$\mathbf{B_{14}}$	$=$	$\left(x_4 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_4 - \frac{1}{2}\right)\mathbf{a_2}$	$=$	$a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}}$	(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
$\mathbf{B_{17}}$	$=$	$-\left(x_5 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_5 + \frac{1}{2}\right)\mathbf{a_2}$	$=$	$-a\left(x_5 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}}$	(4g)	Ru II
$\mathbf{B_{18}}$	$=$	$\left(x_5 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_5 - \frac{1}{2}\right)\mathbf{a_2}$	$=$	$a\left(x_5 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}}$	(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
$\mathbf{B_{21}}$	$=$	$-\left(x_6 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_6 + \frac{1}{2}\right)\mathbf{a_2}$	$=$	$-a\left(x_6 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\hat{\mathbf{y}}$	(4g)	Ru III
$\mathbf{B_{22}}$	$=$	$\left(x_6 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_6 - \frac{1}{2}\right)\mathbf{a_2}$	$=$	$a\left(x_6 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\hat{\mathbf{y}}$	(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
$\mathbf{B_{25}}$	$=$	$-\left(x_7 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_7 + \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{2}\mathbf{a_3}$	$=$	$-a\left(x_7 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	B IV
$\mathbf{B_{26}}$	$=$	$\left(x_7 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_7 - \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{2}\mathbf{a_3}$	$=$	$a\left(x_7 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{28}}$	$=$	$-x_8\,\mathbf{a_1} - y_8\,\mathbf{a_2} + \frac{1}{2}\mathbf{a_3}$	$=$	$-ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Ru IV

$$\mathbf{B_{29}} = -\left(x_8 - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_8 + \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = -a\left(x_8 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_8 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \qquad (4h) \qquad \text{Ru IV}$$

$$\mathbf{B_{30}} = \left(x_8 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_8 - \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = a\left(x_8 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_8 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \qquad (4h) \qquad \text{Ru IV}$$

$$\mathbf{B_{31}} = x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \qquad (4h) \qquad \text{Ru V}$$

$$\mathbf{B_{32}} = -x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = -ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \qquad (4h) \qquad \text{Ru V}$$

$$\mathbf{B_{33}} = -\left(x_9 - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_9 + \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = -a\left(x_9 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_9 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \qquad (4h) \qquad \text{Ru V}$$

$$\mathbf{B_{34}} = \left(x_9 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_9 - \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = a\left(x_9 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_9 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \qquad (4h) \qquad \text{Ru V}$$

$$\mathbf{B_{35}} = x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \qquad (4h) \qquad \text{Ru VI}$$

$$\mathbf{B_{36}} = -x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = -ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \qquad (4h) \qquad \text{Ru VI}$$

$$\mathbf{B_{37}} = -\left(x_{10} - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{10} + \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = -a\left(x_{10} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{10} + \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \qquad (4h) \qquad \text{Ru VI}$$

$$\mathbf{B_{38}} = \left(x_{10} + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_{10} - \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = a\left(x_{10} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{10} - \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \qquad (4h) \qquad \text{Ru VI}$$

References

[1] J. Åselius, *The Crystal Structure of $Ru_{11}B_8$*, Acta Chem. Scand. **14**, 2169–2176 (1960), doi:10.3891/acta.chem.scand.14-2169.