

RuB₂ Structure: A2B_oP6_59_e_a-001

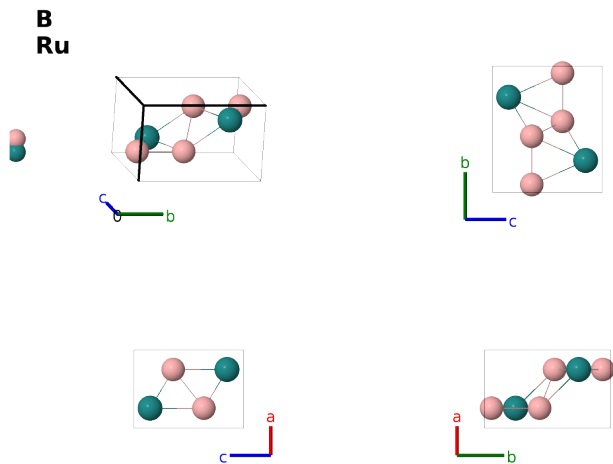
This structure previously used the label(s) **A2B_oP6_59_f_a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/BRW1>

https://aflow.org/prototype-encyclopedia/A2B_oP6_59_e_a-001



Prototype	B ₂ Ru
AFLOW prototype label	A2B_oP6_59_e_a-001
ICSD	615356
CCDC	1746418
Pearson symbol	oP6
Space group number	59
Space group symbol	<i>Pmnm</i>
AFLOW prototype command	<code>aflow --proto=A2B_oP6_59_e_a-001 --params=a, b/a, c/a, z₁, y₂, z₂</code>

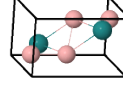
Other compounds with this structure

OsB₂

Simple Orthorhombic primitive vectors



$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2a)	Ru I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(2a)	Ru I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4e)	B I
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4e)	B I
$\mathbf{B}_5$	$= \frac{3}{4} \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4e)	B I
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4e)	B I

References

- [1] B. Aronsson, *The Crystal Structure of RuB_2 , OsB_2 , and $\text{IrB}_{1.35}$ and Some General Comments on the Crystal Chemistry of Borides in the Composition Range MeB - MeB_3* , Acta Chem. Scand. **17**, 2036–2050 (1963), doi:10.3891/acta.chem.scand.17-2036.

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