

Re₃B Structure:

AB3_oC16_63_c_cf-001

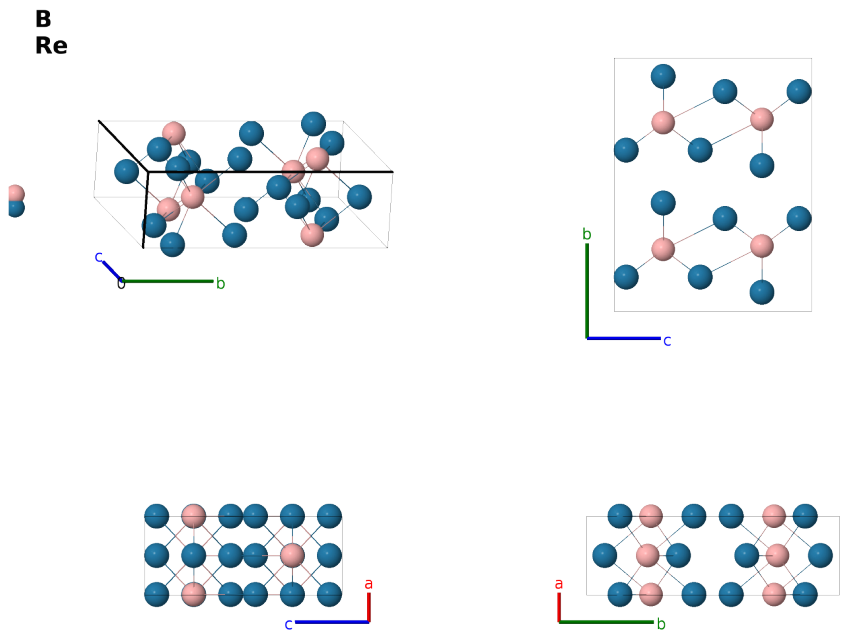
This structure previously used the label(s) **AB3_oC16_63_c_cf**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/EW0Y>

https://aflow.org/prototype-encyclopedia/AB3_oC16_63_c_cf-001



Prototype	BRe ₃
AFLOW prototype label	AB3_oC16_63_c_cf-001
ICSD	43662
CCDC	1613135
Pearson symbol	oC16
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=AB3_oC16_63_c_cf-001</code> <code>--params=a, b/a, c/a, y₁, y₂, y₃, z₃</code>

Other compounds with this structure

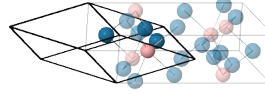
BTc₃, CoPu₃

- This is the parent structure of the ternary MgCuAl₂ (*E1_a*) structure. There are also “filled” versions of this structure, V₃AsC and ThFe₂SiC.
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Base-centered Orthorhombic primitive vectors

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





Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Re I
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Re I
$\mathbf{B}_5$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8f)	Re II
$\mathbf{B}_6$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Re II
$\mathbf{B}_7$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Re II
$\mathbf{B}_8$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8f)	Re II

References

- [1] B. Aronsson, M. Bäckman, and S. Rundqvist, *The Crystal Structure of Re₃B*, Acta Chem. Scand. **14**, 1001–1005 (1960), doi:10.3891/acta.chem.scand.14-1001.

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