

ReB₃ Structure:

A3B_hP8_194_af_c-001

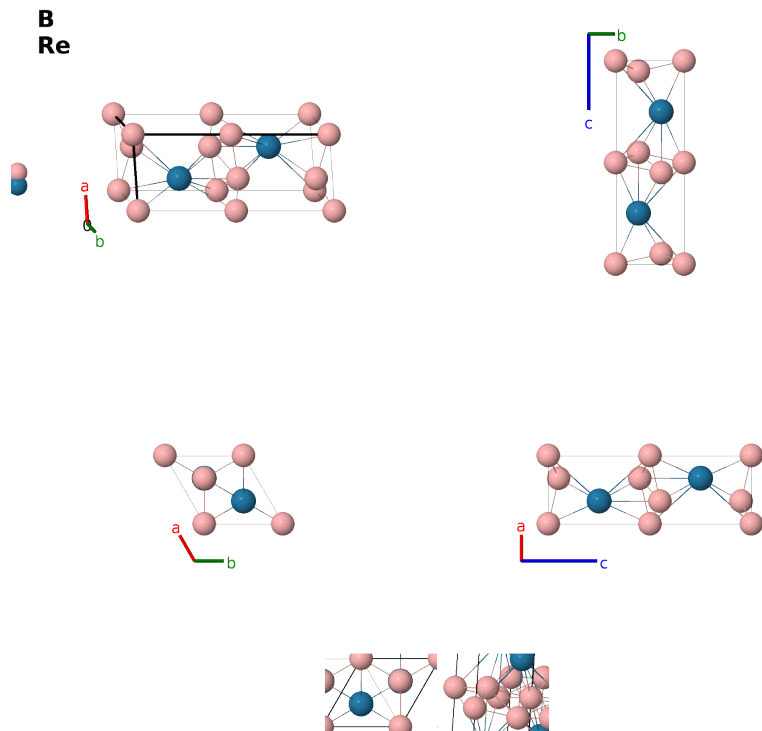
This structure previously used the label(s) **A3B_hP8_194_af_c**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/72PY>

https://aflow.org/prototype-encyclopedia/A3B_hP8_194_af_c-001



Prototype	B ₃ Re
AFLOW prototype label	A3B_hP8_194_af_c-001
ICSD	24361
CCDC	1600401
Pearson symbol	hP8
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=A3B_hP8_194_af_c-001</code> <code>--params=a,c/a,z₃</code>

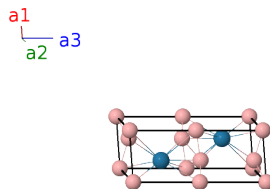
Other compounds with this structure

TcB₃, CaNi₂Si, GdPt₂Sn

- The lattice constants a and c were inferred from the nearest-neighbor distances in (Aronsson, 1960).
 - (Frotscher, 2010) states that this structure was “falsely assigned,” and that the true structure is ReB₂, which is identical to this structure with the (2a) boron atoms removed.
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Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(2a) B I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(2a) B I
$\mathbf{B}_3$	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c) Re I
$\mathbf{B}_4$	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c) Re I
$\mathbf{B}_5$	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4f) B II
$\mathbf{B}_6$	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f) B II
$\mathbf{B}_7$	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4f) B II
$\mathbf{B}_8$	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f) B II

References

- [1] B. Aronsson, E. Stenberg, and J. Åselius, *Borides of Rhenium and the Platinum Metals*, Acta Chem. Scand. **14**, 733–741 (1960), doi:10.3891/acta.chem.scand.14-0733.
- [2] M. Frotscher, M. Hölzel, and B. Albert, *Crystal Structures of the Metal Diborides ReB₂, RuB₂, and OsB₂ from Neutron Powder Diffraction*, Z. Anorganische und Allgemeine Chemie **636**, 1783–1786 (2010), doi:10.1002/zaac.201000101.

Found in

- [1] P. Villars and L. Calvert, *Pearson’s Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OK, 1991), vol. I, chap. , p. 612.

First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.