

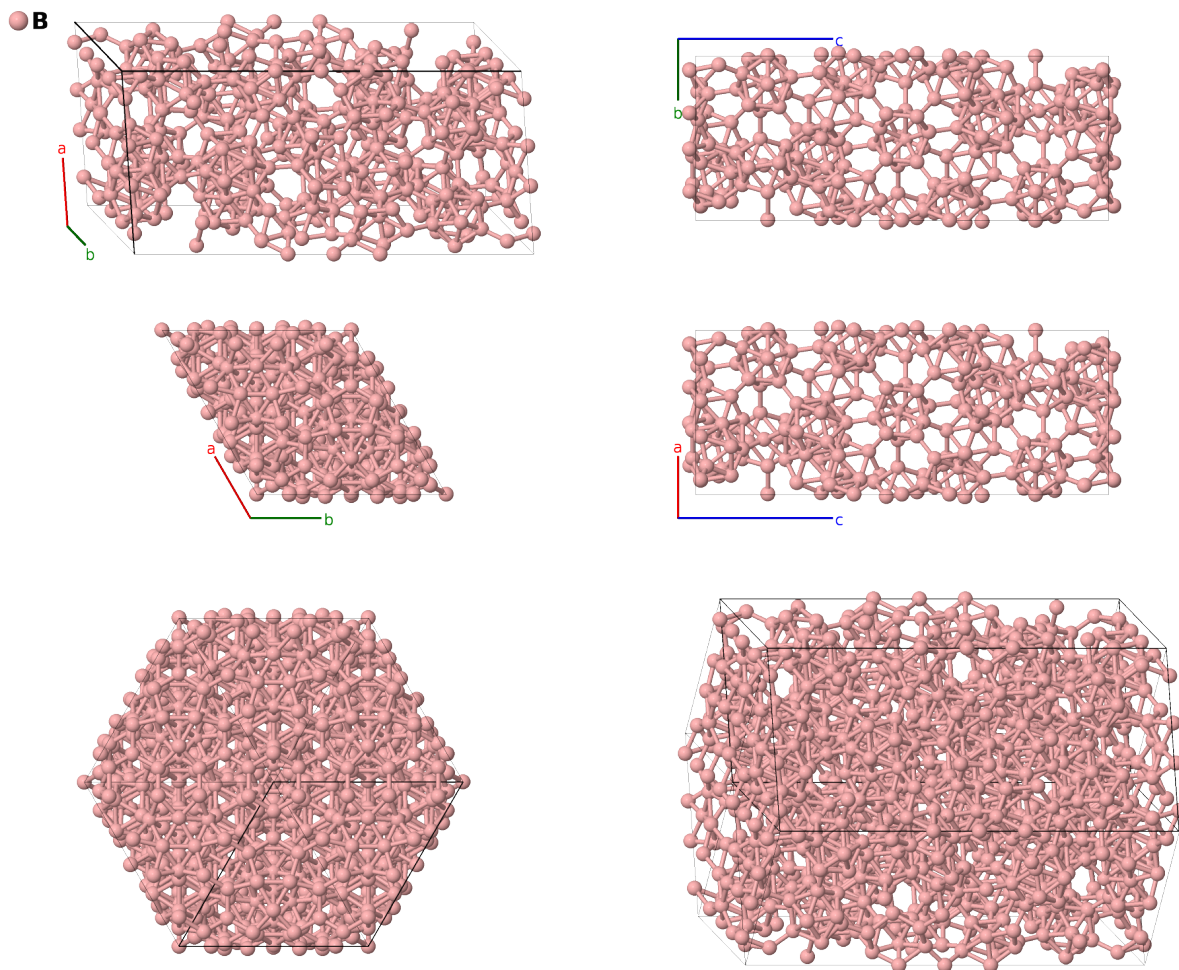
β -B (R-105) Structure: A_hR105_166_ac9h4i-001

This structure originally had the label A_hR105_166_bc9h4i. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

<https://aflow.org/p/Y6TF>

https://aflow.org/p/A_hR105_166_ac9h4i-001



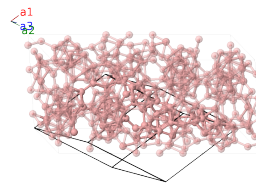
Prototype	B
AFLOW prototype label	A_hR105_166_ac9h4i-001
ICSD	14288
Pearson symbol	hR105
Space group number	166
Space group symbol	$R\bar{3}m$

AFLOW prototype command `aflow --proto=A_hr105_166_ac9h4i-001`
`--params=a, c/a, x2, x3, z3, x4, z4, x5, z5, x6, z6, x7, z7, x8, z8, x9, z9, x10, z10, x11, z11, x12, y12, z12, x13, y13, z13, x14, y14, z14, x15, y15, z15`

- This is apparently the ground state of boron, with 105 atoms in the unit cell.
- (Donohue, 1982) gives two possible sets of internal coordinates for the atoms on page 64. We use the second set (Geist, 1970), as it has no partially filled sites.
- Note the relationship between the icosahedra in this structure, α -B and T-50 B.
- Hexagonal settings for rhombohedral structures can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(1a)	B I
\mathbf{B}_2	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(2c)	B II
\mathbf{B}_3	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-cx_2 \hat{\mathbf{z}}$	(2c)	B II
\mathbf{B}_4	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(6h)	B III
\mathbf{B}_5	$z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(6h)	B III
\mathbf{B}_6	$x_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(6h)	B III
\mathbf{B}_7	$-z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(6h)	B III
\mathbf{B}_8	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(6h)	B III
\mathbf{B}_9	$-x_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$\frac{1}{\sqrt{3}}a(x_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(6h)	B III
\mathbf{B}_{10}	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	B IV
\mathbf{B}_{11}	$z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	B IV
\mathbf{B}_{12}	$x_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	B IV
\mathbf{B}_{13}	$-z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	B IV
\mathbf{B}_{14}	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	B IV
\mathbf{B}_{15}	$-x_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$\frac{1}{\sqrt{3}}a(x_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(2x_4 + z_4) \hat{\mathbf{z}}$	(6h)	B IV
\mathbf{B}_{16}	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h)	B V

$$\begin{aligned}
\mathbf{B}_{98} &= -y_{15} \mathbf{a}_1 - x_{15} \mathbf{a}_2 - z_{15} \mathbf{a}_3 &= & -\frac{1}{2}a (y_{15} - z_{15}) \hat{\mathbf{x}} - & (12i) & \text{B XV} \\
&&& \frac{\sqrt{3}}{6}a (2x_{15} - y_{15} - z_{15}) \hat{\mathbf{y}} - \\
&&& \frac{1}{3}c (x_{15} + y_{15} + z_{15}) \hat{\mathbf{z}} \\
\mathbf{B}_{99} &= -x_{15} \mathbf{a}_1 - z_{15} \mathbf{a}_2 - y_{15} \mathbf{a}_3 &= & -\frac{1}{2}a (x_{15} - y_{15}) \hat{\mathbf{x}} + & (12i) & \text{B XV} \\
&&& \frac{\sqrt{3}}{6}a (x_{15} + y_{15} - 2z_{15}) \hat{\mathbf{y}} - \\
&&& \frac{1}{3}c (x_{15} + y_{15} + z_{15}) \hat{\mathbf{z}} \\
\mathbf{B}_{100} &= -x_{15} \mathbf{a}_1 - y_{15} \mathbf{a}_2 - z_{15} \mathbf{a}_3 &= & -\frac{1}{2}a (x_{15} - z_{15}) \hat{\mathbf{x}} + & (12i) & \text{B XV} \\
&&& \frac{\sqrt{3}}{6}a (x_{15} - 2y_{15} + z_{15}) \hat{\mathbf{y}} - \\
&&& \frac{1}{3}c (x_{15} + y_{15} + z_{15}) \hat{\mathbf{z}} \\
\mathbf{B}_{101} &= -z_{15} \mathbf{a}_1 - x_{15} \mathbf{a}_2 - y_{15} \mathbf{a}_3 &= & \frac{1}{2}a (y_{15} - z_{15}) \hat{\mathbf{x}} - & (12i) & \text{B XV} \\
&&& \frac{\sqrt{3}}{6}a (2x_{15} - y_{15} - z_{15}) \hat{\mathbf{y}} - \\
&&& \frac{1}{3}c (x_{15} + y_{15} + z_{15}) \hat{\mathbf{z}} \\
\mathbf{B}_{102} &= -y_{15} \mathbf{a}_1 - z_{15} \mathbf{a}_2 - x_{15} \mathbf{a}_3 &= & \frac{1}{2}a (x_{15} - y_{15}) \hat{\mathbf{x}} + & (12i) & \text{B XV} \\
&&& \frac{\sqrt{3}}{6}a (x_{15} + y_{15} - 2z_{15}) \hat{\mathbf{y}} - \\
&&& \frac{1}{3}c (x_{15} + y_{15} + z_{15}) \hat{\mathbf{z}} \\
\mathbf{B}_{103} &= z_{15} \mathbf{a}_1 + y_{15} \mathbf{a}_2 + x_{15} \mathbf{a}_3 &= & -\frac{1}{2}a (x_{15} - z_{15}) \hat{\mathbf{x}} - & (12i) & \text{B XV} \\
&&& \frac{\sqrt{3}}{6}a (x_{15} - 2y_{15} + z_{15}) \hat{\mathbf{y}} + \\
&&& \frac{1}{3}c (x_{15} + y_{15} + z_{15}) \hat{\mathbf{z}} \\
\mathbf{B}_{104} &= y_{15} \mathbf{a}_1 + x_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3 &= & \frac{1}{2}a (y_{15} - z_{15}) \hat{\mathbf{x}} + & (12i) & \text{B XV} \\
&&& \frac{\sqrt{3}}{6}a (2x_{15} - y_{15} - z_{15}) \hat{\mathbf{y}} + \\
&&& \frac{1}{3}c (x_{15} + y_{15} + z_{15}) \hat{\mathbf{z}} \\
\mathbf{B}_{105} &= x_{15} \mathbf{a}_1 + z_{15} \mathbf{a}_2 + y_{15} \mathbf{a}_3 &= & \frac{1}{2}a (x_{15} - y_{15}) \hat{\mathbf{x}} - & (12i) & \text{B XV} \\
&&& \frac{\sqrt{3}}{6}a (x_{15} + y_{15} - 2z_{15}) \hat{\mathbf{y}} + \\
&&& \frac{1}{3}c (x_{15} + y_{15} + z_{15}) \hat{\mathbf{z}}
\end{aligned}$$

References

- [1] D. Geist, R. Kloss, and H. Follner, *Verfeinerung des β -rhomboedrischen Bors*, Acta Crystallogr. Sect. B **26**, 1800–1804 (1970), doi:10.1107/S0567740870004910.

Found in

- [1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).