α-B (R-12) Structure: A_hR12_166_2h-001

This structure previously used the label(s) `A_hR12_166_2h`. Calls to these addresses will be redirected here.

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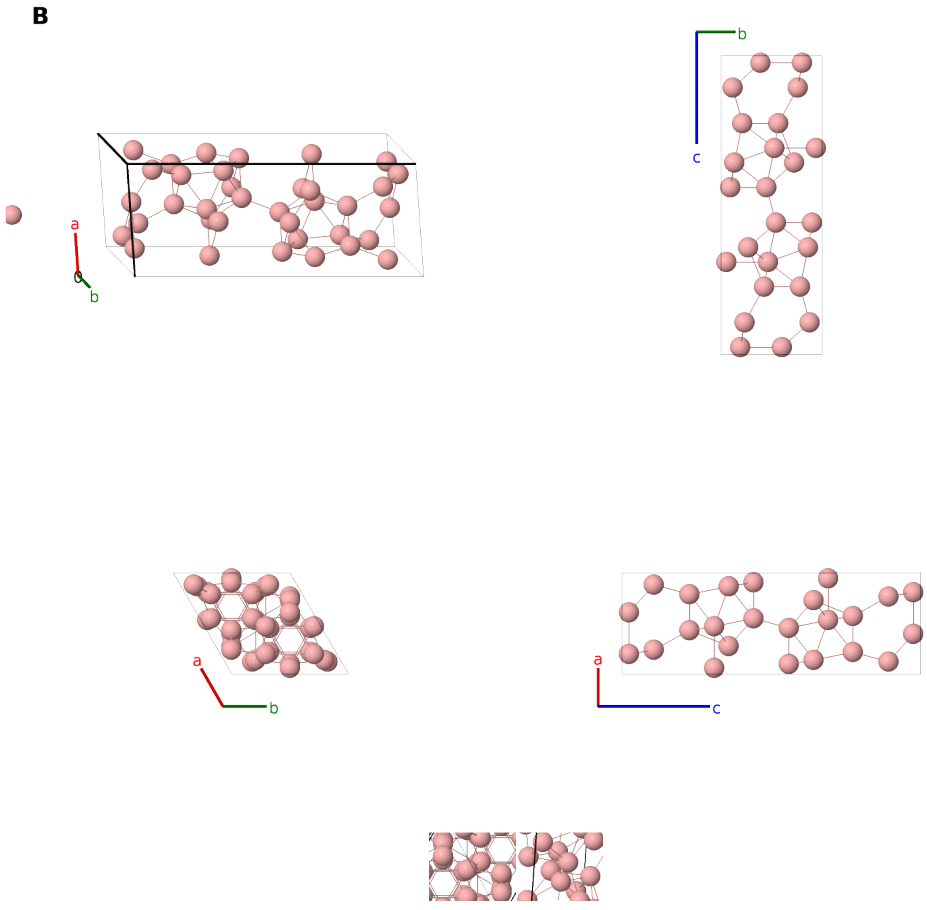
https://aflow.org/prototype-encyclopedia/1Y2H

https://aflow.org/prototype-encyclopedia/A_hR12_166_2h-001



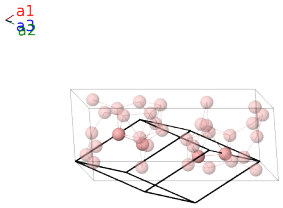
Prototype	B
AFLOW prototype label	A_hR12_166_2h-001
ICSD	26487
CCDC	1601887
Pearson symbol	hR12
Space group number	166
Space group symbol	$R\bar{3}m$

AFLOW prototype command `aflow --proto=A_hR12_166_2h-001 --params=`$a, c/a, x_1, z_1, x_2, z_2$

- This is a metastable phase of boron, also known as rhombohedral-12 boron (Donohue, 1982). It is the simplest known phase (the ground state, β-B, has 105 atoms in the primitive cell).
- Note the relationship between the icosahedra in this structure, β-B and T-50 B.
- Hexagonal settings for rhombohedral structures can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1 - z_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_1 - z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_1 + z_1)\,\hat{\mathbf{z}}$	(6h)	B I
$\mathbf{B_2}$	=	$z_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_1 - z_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_1 - z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_1 + z_1)\,\hat{\mathbf{z}}$	(6h)	B I
$\mathbf{B_3}$	=	$x_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_1 - z_1)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_1 + z_1)\,\hat{\mathbf{z}}$	(6h)	B I
$\mathbf{B_4}$	=	$-z_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1 - z_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_1 - z_1)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_1 + z_1)\,\hat{\mathbf{z}}$	(6h)	B I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_1 - z_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_1 - z_1)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_1 + z_1)\,\hat{\mathbf{z}}$	(6h)	B I
$\mathbf{B_6}$	=	$-x_1\,\mathbf{a}_1 - z_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_1 - z_1)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_1 + z_1)\,\hat{\mathbf{z}}$	(6h)	B I
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(6h)	B II
$\mathbf{B_8}$	=	$z_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(6h)	B II
$\mathbf{B_9}$	=	$x_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(6h)	B II
$\mathbf{B_{10}}$	=	$-z_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_2 - z_2)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(6h)	B II
$\mathbf{B_{11}}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_2 - z_2)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(6h)	B II
$\mathbf{B_{12}}$	=	$-x_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_2 - z_2)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(6h)	B II

References

[1] B. F. Decker and J. S. Kasper, *The crystal structure of a simple rhombohedral form of boron*, Acta Cryst. **12**, 503–506 (1959), doi:10.1107/S0365110X59001529.

Found in

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

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. 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