

BN (B_k) Structure: AB_hP4_194_c_d-001

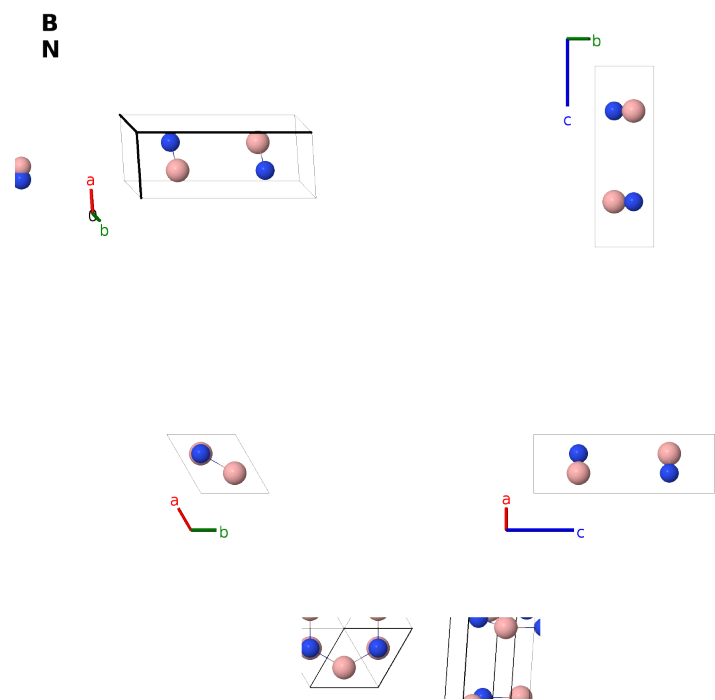
This structure previously used the label(s) **AB_hP4_194_c_d**. Calls to these addresses will be redirected here.

Cite this page as:

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

https://aflow.org/prototype-encyclopedia/AB_hP4_194_c_d-001



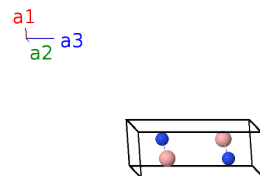
Prototype	BN
AFLOW prototype label	AB_hP4_194_c_d-001
<i>Strukturbericht</i> designation	B_k
ICSD	24644
CCDC	1600662
Pearson symbol	hP4
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=AB_hP4_194_c_d-001 --params=a, c/a</code>

Other compounds with this structure

ZnO nanowires

- This is the corrected boron nitride structure found by (Pease, 1950) and (Pease, 1952). See further discussion on the *B12* page.
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Hexagonal primitive vectors

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


The diagram shows the three primitive vectors $\mathbf{a}_1$ (red), $\mathbf{a}_2$ (green), and $\mathbf{a}_3$ (blue) originating from a common point. $\mathbf{a}_1$ and $\mathbf{a}_2$ are in the xy-plane, while $\mathbf{a}_3$ is along the z-axis. To the right, a 3D rectangular unit cell is shown with four spheres (two red, two blue) representing atoms at the corners.

Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(2c)	B I
$\mathbf{B}_2$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(2c)	B I
$\mathbf{B}_3$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(2d)	N I
$\mathbf{B}_4$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(2d)	N I

References

- [1] R. S. Pease, *Crystal Structure of Boron Nitride*, Nature **165**, 722–723 (1950), doi:10.1038/165722b0.
- [2] R. S. Pease, *An X-ray study of boron nitride*, Acta Cryst. **5**, 356–361 (1952), doi:10.1107/S0365110X52001064.

Found in

- [1] R. G. W. Wyckoff, *Crystal Structure*, vol. 1 (Interscience, New York, London, Sydney, 1963).

First cited in

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