BN (B_k) Structure: AB_hP4_194_c_d-001

This structure originally had the label `AB_hP4_194_c_d`. Calls to that address will be redirected here.

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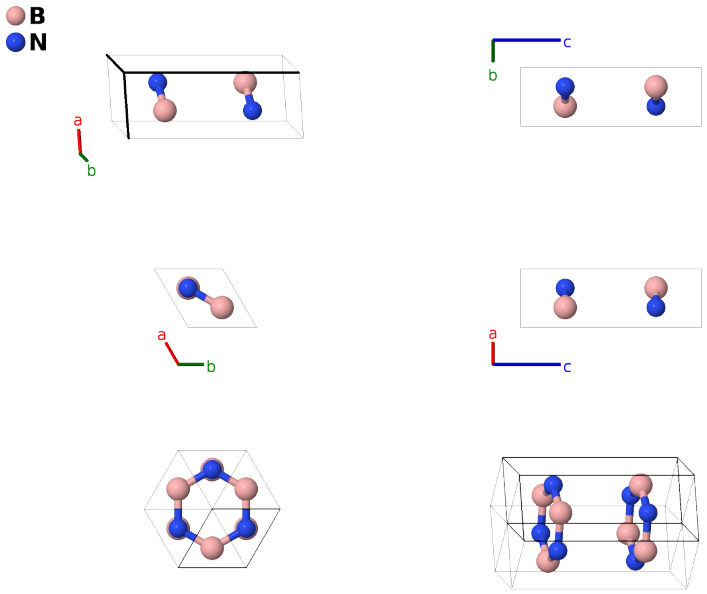
https://aflow.org/p/SHYT

https://aflow.org/p/AB_hP4_194_c_d-001



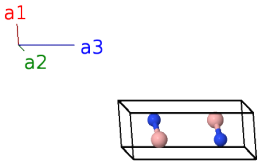
Prototype	BN
AFLOW prototype label	AB_hP4_194_c_d-001
***Strukturbericht* designation**	B_k
ICSD	24644
Pearson symbol	hP4
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=AB_hP4_194_c_d-001 --params=`$a, c/a$

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.

Hexagonal primitive vectors

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



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).