Original BN ($B12$) Structure (*Obsolete*): AB_hP4_186_b_a-001

This structure previously used the label(s) `AB_hP4_186_b_a`. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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.

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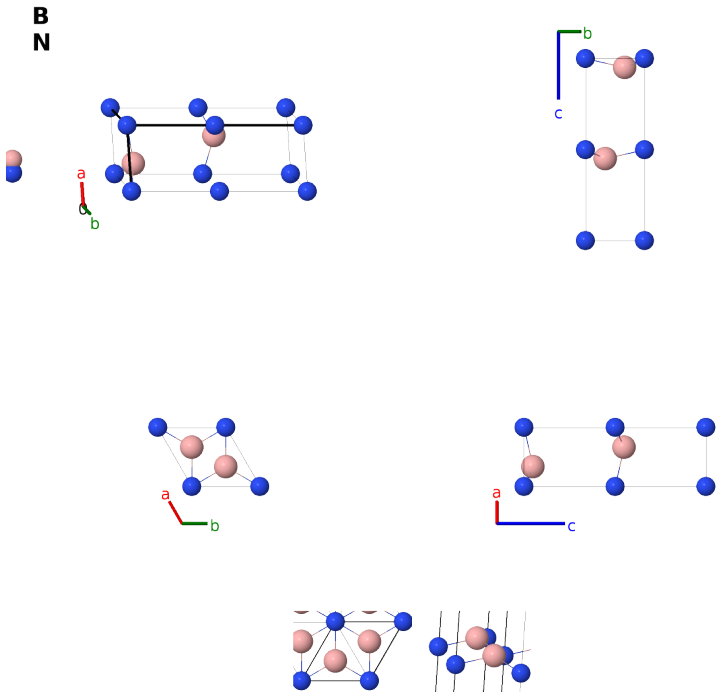
https://aflow.org/prototype-encyclopedia/QUDC

https://aflow.org/prototype-encyclopedia/AB_hP4_186_b_a-001

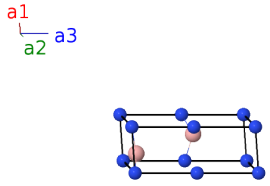


Prototype	BN
AFLOW prototype label	AB_hP4_186_b_a-001
***Strukturbericht* designation**	$B12$
ICSD	77374
CCDC	1637806
Pearson symbol	hP4
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	`aflow --proto=AB_hP4_186_b_a-001 --params=`$a, c/a, z_1, z_2$

- This is the BN structure found in (Ewald, 1931) p. 95 and (Wilson, 1961) pp. 125-126. (Pease, 1950) later determined that the true boron nitride structure is what is now known as the B_k structure. We leave this structure here for historical reasons. It is crystallographically equivalent to, and hence a binary representation of, the buckled graphite structure.
- Space group $P6_3$ #186 is polar, so there is no fixed origin for the z axis. Here we chose $z_1 = 0$ for the boron (2a) site.

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
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	N I
$\mathbf{B_2}$	=	$\left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	N I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2b)	B I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	B I

References

[1] A. Brager, *X-ray examination of the structure of boron nitride*, Acta Physicochimica URSS **7**, 699–706 (1937).

[2] R. S. Pease, *Crystal Structure of Boron Nitride*, Nature **165**, 722–723 (1950), doi:10.1038/165722b0.

[3] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).

Found in

[1] A. J. C. Wilson, ed., *Structure Reports for 1947–1948*, *Structure Reports*, vol. 18 (N.V.A. Oosthoek's Uitgevers, Utrecht, 1961).

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