

BN (High-pressure, high-temperature) Structure: AB_oF8_42_a_a-001

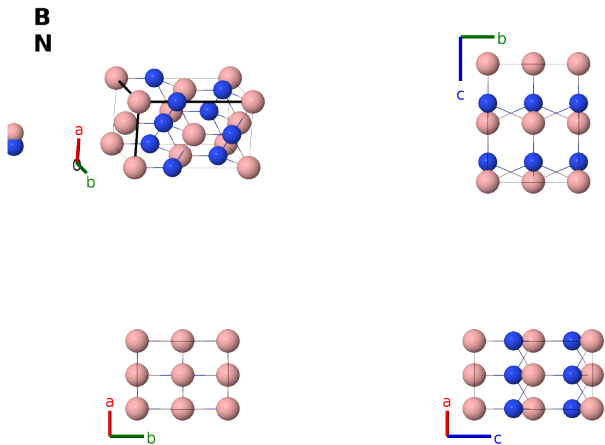
This structure previously used the label(s) **AB_oF8_42_a_a**. Calls to these addresses will be redirected here.

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.

<https://aflow.org/prototype-encyclopedia/0Q2T>

https://aflow.org/prototype-encyclopedia/AB_oF8_42_a_a-001

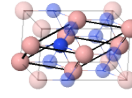


Prototype	BN
AFLOW prototype label	AB_oF8_42_a_a-001
ICSD	20946
CCDC	1598669
Pearson symbol	oF8
Space group number	42
Space group symbol	<i>Fmm2</i>
AFLOW prototype command	<code>aflow --proto=AB_oF8_42_a_a-001 --params=a, b/a, c/a, z₁, z₂</code>

Face-centered Orthorhombic primitive vectors



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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(4a)	B I
$\mathbf{B}_2$	$= z_2 \mathbf{a}_1 + z_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(4a)	N I

References

- [1] A. V. Kurdyumov and G. S. Olejnik, *On metastable structures of graphite-like boron nitride*, Kristallografiya **29**, 792–793 (1984).

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

- D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043