

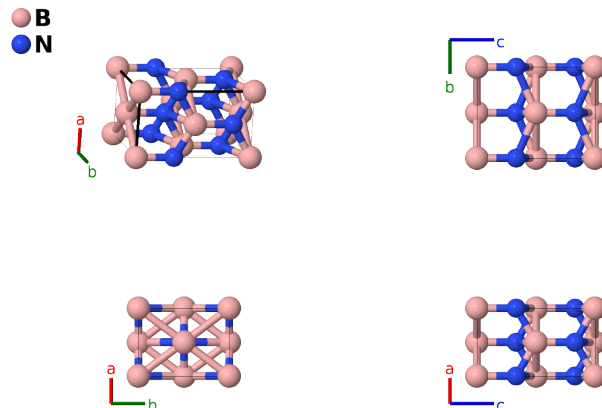
# BN (High-pressure, high-temperature) Structure: AB\_oF8\_42\_a\_a-001

This structure originally had the label AB\_oF8\_42\_a\_a. Calls to that address will be redirected here.

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<https://afLOW.org/p/0Q2T>

[https://afLOW.org/p/AB\\_oF8\\_42\\_a\\_a-001](https://afLOW.org/p/AB_oF8_42_a_a-001)



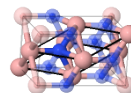
Prototype	BN
AFLOW prototype label	AB_oF8_42_a_a-001
ICSD	20946
Pearson symbol	oF8
Space group number	42
Space group symbol	<i>Fmm2</i>
AFLOW prototype command	afLOW --proto=AB_oF8_42_a_a-001 --params=a, b/a, c/a, z <sub>1</sub> , z <sub>2</sub>

## Face-centered Orthorhombic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}b\hat{y} + \frac{1}{2}c\hat{z}$$

$$\mathbf{a}_2 = \frac{1}{2}a\hat{x} + \frac{1}{2}c\hat{z}$$

$$\mathbf{a}_3 = \frac{1}{2}a\hat{x} + \frac{1}{2}b\hat{y}$$



## 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.