

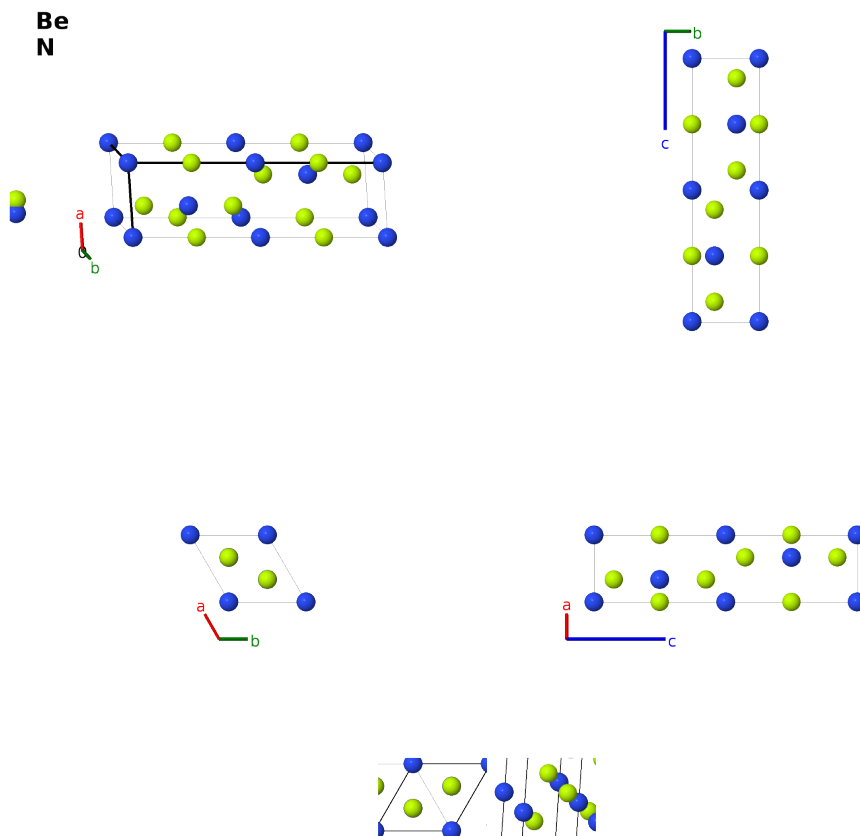
β -Be₃N₂ Structure: A3B2_hP10_194_bf_ac-001

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

https://aflow.org/prototype-encyclopedia/A3B2_hP10_194_bf_ac-001

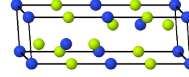


Prototype	Be ₃ N ₂
AFLOW prototype label	A3B2_hP10_194_bf_ac-001
ICSD	25656
CCDC	1601305
Pearson symbol	hP10
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=A3B2_hP10_194_bf_ac-001 --params=a, c/a, z₄</code>

- This is the high-temperature structure of Be_3N_2 . Below 1270°C $\alpha\text{-Be}_3\text{N}_2$ is in the cubic bixbyite ($D5_3$) structure (Wriedt, 1987).

Hexagonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(2a)	N I
$\mathbf{B}_2$	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}c\hat{\mathbf{z}}$	(2a)	N I
$\mathbf{B}_3$	$\frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}c\hat{\mathbf{z}}$	(2b)	Be I
$\mathbf{B}_4$	$\frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}c\hat{\mathbf{z}}$	(2b)	Be I
$\mathbf{B}_5$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(2c)	N II
$\mathbf{B}_6$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(2c)	N II
$\mathbf{B}_7$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + z_4\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(4f)	Be II
$\mathbf{B}_8$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + (z_4 + \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + c(z_4 + \frac{1}{2})\hat{\mathbf{z}}$	(4f)	Be II
$\mathbf{B}_9$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 - z_4\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(4f)	Be II
$\mathbf{B}_{10}$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 - (z_4 - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - c(z_4 - \frac{1}{2})\hat{\mathbf{z}}$	(4f)	Be II

References

- [1] P. Eckerlin and A. Rabenau, *Zur Kenntnis des Systems $\text{Be}_3\text{N}_2\text{-Si}_3\text{N}_4$ Die Struktur einer neuen Modifikation von Be_3N_2* , Z. Anorganische und Allgemeine Chemie **218**, 218–229 (1960), doi:10.1002/zaac.19603040313.

Found in

- [1] H. A. Wriedt and H. Okamoto, *The BeN (Beryllium-Nitrogen) system*, J. Phase Equilibria **8**, 136–139 (1987), doi:10.1007/BF02873199.

First cited in

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