

Theoretical cI24 AlN Structure: AB_cI24_220_a_b-001

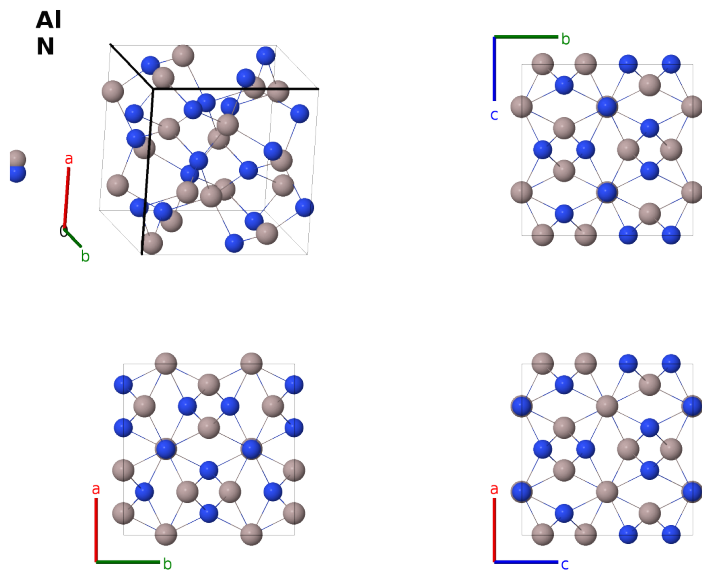
This structure previously used the label(s) **AB_cI24_220_a_b**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/MH9E>

https://aflow.org/prototype-encyclopedia/AB_cI24_220_a_b-001

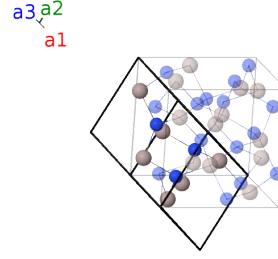


Prototype	AlN
AFLOW prototype label	AB.cI24_220_a_b-001
Pearson symbol	cI24
Space group number	220
Space group symbol	$I\bar{4}3d$
AFLOW prototype command	<code>aflow --proto=AB_cI24_220_a_b-001 --params=a</code>

- AlN naturally occurs in two forms (Liu, 2019): the stable wz-AlN wurtzite ($B4$) structure, and the high-pressure rs-AlN rock salt ($B1$) structure. A metastable zb-AlN zincblende (zb-AlN) structure can be synthesized via a solid-state reaction.
- (Liu, 2019) used a first-principles evolutionary technique to find four possible metastable phases: one in the sc16 structure, and three novel cubic structures, cF40, cI16, and cI24.

Body-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{3}{8}\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(12a)	Al I
$\mathbf{B}_2$	$= \frac{3}{4}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{1}{8}\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{z}}$	(12a)	Al I
$\mathbf{B}_3$	$= \frac{3}{8}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{5}{8}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{3}{8}a\hat{\mathbf{y}}$	(12a)	Al I
$\mathbf{B}_4$	$= \frac{1}{8}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{7}{8}\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}}$	(12a)	Al I
$\mathbf{B}_5$	$= \frac{5}{8}\mathbf{a}_1 + \frac{3}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(12a)	Al I
$\mathbf{B}_6$	$= \frac{7}{8}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(12a)	Al I
$\mathbf{B}_7$	$= \frac{1}{4}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{7}{8}\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{4}a\hat{\mathbf{z}}$	(12b)	N I
$\mathbf{B}_8$	$= \frac{3}{4}\mathbf{a}_1 + \frac{3}{8}\mathbf{a}_2 + \frac{5}{8}\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(12b)	N I
$\mathbf{B}_9$	$= \frac{7}{8}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{8}\mathbf{a}_3$	$=$	$-\frac{1}{4}a\hat{\mathbf{x}} + \frac{3}{8}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(12b)	N I
$\mathbf{B}_{10}$	$= \frac{5}{8}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{3}{8}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(12b)	N I
$\mathbf{B}_{11}$	$= \frac{1}{8}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(12b)	N I
$\mathbf{B}_{12}$	$= \frac{3}{8}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(12b)	N I

References

- [1] C. Liu, M. Chen, J. Li, L. Liu, P. Li, M. Ma, C. Shao, J. He, and T. Liang, *A first-principles study of novel cubic AlN phases* **130**, 58–66 (2019), doi:10.1016/j.jpcs.2019.02.009.

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