

Theoretical cI16 AlN Structure: AB_cI16_217_c_c-001

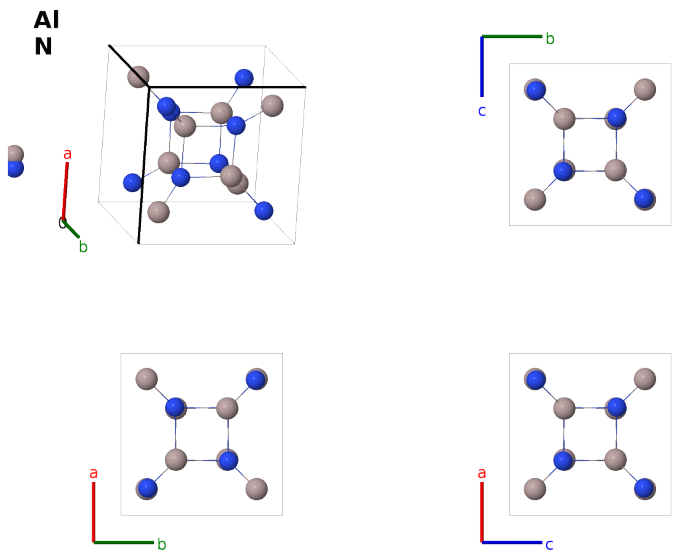
This structure previously used the label(s) **AB_cI16_217_c_c**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/6RJH>

https://aflow.org/prototype-encyclopedia/AB_cI16_217_c_c-001

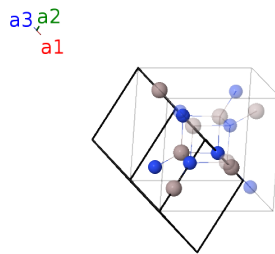


Prototype	AlN
AFLOW prototype label	AB_cI16_217_c_c-001
Pearson symbol	cI16
Space group number	217
Space group symbol	$I\bar{4}3m$
AFLOW prototype command	<code>aflow --proto=AB_cI16_217_c_c-001</code> <code>--params=a, x_1, x_2</code>

- 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 (*B3*) 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 (this structure), 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
$\mathbf{B}_1$	$= 2x_1 \mathbf{a}_1 + 2x_1 \mathbf{a}_2 + 2x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(8c)	Al I
$\mathbf{B}_2$	$= -2x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(8c)	Al I
$\mathbf{B}_3$	$= -2x_1 \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(8c)	Al I
$\mathbf{B}_4$	$= -2x_1 \mathbf{a}_1$	$=$	$ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(8c)	Al I
$\mathbf{B}_5$	$= 2x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + 2x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B}_6$	$= -2x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B}_7$	$= -2x_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B}_8$	$= -2x_2 \mathbf{a}_1$	$=$	$ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8c)	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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