$NaAlB_{14}$ Structure: AB14C_oI64_74_c_3h2j_e-001

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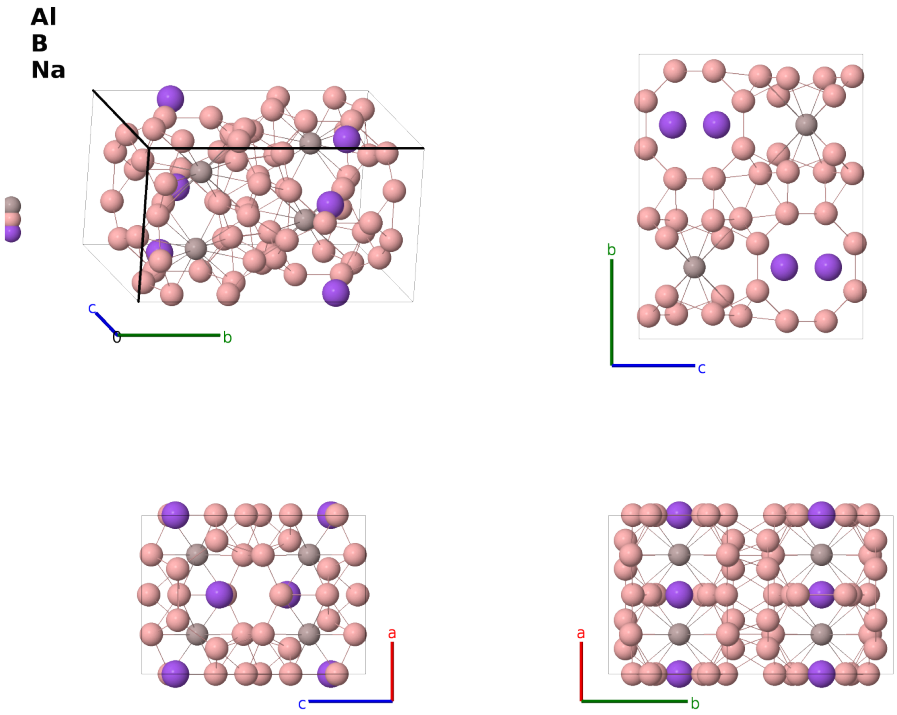
https://aflow.org/prototype-encyclopedia/XE01

https://aflow.org/prototype-encyclopedia/AB14C_oI64_74_c_3h2j_e-001

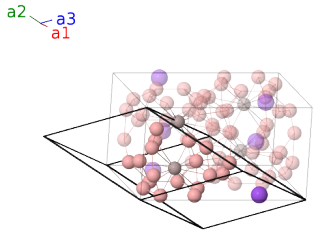


Prototype	$AlB_{14}Na$
AFLOW prototype label	AB14C_oI64_74_c_3h2j_e-001
ICSD	152701
CCDC	1669426
Pearson symbol	oI64
Space group number	74
Space group symbol	$Imma$
AFLOW prototype command	`aflow --proto=AB14C_oI64_74_c_3h2j_e-001 --params=`$a, b/a, c/a, z_2, y_3, z_3, y_4, z_4, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

- The stoichiometry of this sample is given as $Na_{0.95}Al_{0.94}B_{14}$, indicating vacancies on the sodium and aluminum sites.
- (Okada, 2005) say that this is isomorphous to $MgAlB_{14}$, but our published version of that structure has the Mg site split, rather than a single Na site.
- The AFLOW prototype label protocol swaps the a and b lattice constants, and moves the origin by 1/4 a $\hat{x}$ + 1/4 b $\hat{y}$ + 1/4 c $\hat{z}$, moving the aluminum atom from the published (4b) Wyckoff position to (4c).

Body-centered Orthorhombic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B_3}$	=	$\left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4e)	Na I
$\mathbf{B_4}$	=	$-\left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4e)	Na I
$\mathbf{B_5}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8h)	B I
$\mathbf{B_6}$	=	$\left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8h)	B I
$\mathbf{B_7}$	=	$\left(y_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8h)	B I
$\mathbf{B_8}$	=	$-\left(y_3 + z_3\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8h)	B I
$\mathbf{B_9}$	=	$(y_4 + z_4)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8h)	B II
$\mathbf{B_{10}}$	=	$\left(-y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8h)	B II
$\mathbf{B_{11}}$	=	$\left(y_4 - z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8h)	B II
$\mathbf{B_{12}}$	=	$-\left(y_4 + z_4\right)\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8h)	B II
$\mathbf{B_{13}}$	=	$(y_5 + z_5)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8h)	B III
$\mathbf{B_{14}}$	=	$\left(-y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-b\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8h)	B III
$\mathbf{B_{15}}$	=	$\left(y_5 - z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8h)	B III
$\mathbf{B_{16}}$	=	$-\left(y_5 + z_5\right)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - y_5\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8h)	B III
$\mathbf{B_{17}}$	=	$(y_6 + z_6)\,\mathbf{a}_1 + (x_6 + z_6)\,\mathbf{a}_2 + (x_6 + y_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(16j)	B IV

$$\mathbf{B_{18}} = \left(-y_6 + z_6 + \tfrac{1}{2}\right)\mathbf{a}_1 - (x_6 - z_6)\,\mathbf{a}_2 - \left(x_6 + y_6 - \tfrac{1}{2}\right)\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} - b\left(y_6 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad (16j) \quad \text{B IV}$$

$$\mathbf{B_{19}} = \left(y_6 - z_6 + \tfrac{1}{2}\right)\mathbf{a}_1 - (x_6 + z_6)\,\mathbf{a}_2 + \left(-x_6 + y_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} + b\left(y_6 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad (16j) \quad \text{B IV}$$

$$\mathbf{B_{20}} = -(y_6 + z_6)\,\mathbf{a}_1 + (x_6 - z_6)\,\mathbf{a}_2 + (x_6 - y_6)\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad (16j) \quad \text{B IV}$$

$$\mathbf{B_{21}} = -(y_6 + z_6)\,\mathbf{a}_1 - (x_6 + z_6)\,\mathbf{a}_2 - (x_6 + y_6)\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad (16j) \quad \text{B IV}$$

$$\mathbf{B_{22}} = \left(y_6 - z_6 + \tfrac{1}{2}\right)\mathbf{a}_1 + (x_6 - z_6)\,\mathbf{a}_2 + \left(x_6 + y_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} + b\left(y_6 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad (16j) \quad \text{B IV}$$

$$\mathbf{B_{23}} = \left(-y_6 + z_6 + \tfrac{1}{2}\right)\mathbf{a}_1 + (x_6 + z_6)\,\mathbf{a}_2 + \left(x_6 - y_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} - b\left(y_6 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad (16j) \quad \text{B IV}$$

$$\mathbf{B_{24}} = (y_6 + z_6)\,\mathbf{a}_1 - (x_6 - z_6)\,\mathbf{a}_2 - (x_6 - y_6)\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad (16j) \quad \text{B IV}$$

$$\mathbf{B_{25}} = (y_7 + z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + (x_7 + y_7)\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{B V}$$

$$\mathbf{B_{26}} = \left(-y_7 + z_7 + \tfrac{1}{2}\right)\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - \left(x_7 + y_7 - \tfrac{1}{2}\right)\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} - b\left(y_7 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{B V}$$

$$\mathbf{B_{27}} = \left(y_7 - z_7 + \tfrac{1}{2}\right)\mathbf{a}_1 - (x_7 + z_7)\,\mathbf{a}_2 + \left(-x_7 + y_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} + b\left(y_7 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{B V}$$

$$\mathbf{B_{28}} = -(y_7 + z_7)\,\mathbf{a}_1 + (x_7 - z_7)\,\mathbf{a}_2 + (x_7 - y_7)\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{B V}$$

$$\mathbf{B_{29}} = -(y_7 + z_7)\,\mathbf{a}_1 - (x_7 + z_7)\,\mathbf{a}_2 - (x_7 + y_7)\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{B V}$$

$$\mathbf{B_{30}} = \left(y_7 - z_7 + \tfrac{1}{2}\right)\mathbf{a}_1 + (x_7 - z_7)\,\mathbf{a}_2 + \left(x_7 + y_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} + b\left(y_7 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{B V}$$

$$\mathbf{B_{31}} = \left(-y_7 + z_7 + \tfrac{1}{2}\right)\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + \left(x_7 - y_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} - b\left(y_7 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{B V}$$

$$\mathbf{B_{32}} = (y_7 + z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - (x_7 - y_7)\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{B V}$$

References

[1] S. Okada, T. Tanaka, A. Sato, T. Shishido, K. Kudou, K. Nakajima, and T. Lundström, *Crystal growth and structure refinement of a new higher boride $NaAlB_{14}$*, J. Alloys Compd. **395**, 231–235 (2005), doi:10.1016/j.jallcom.2004.10.057.

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