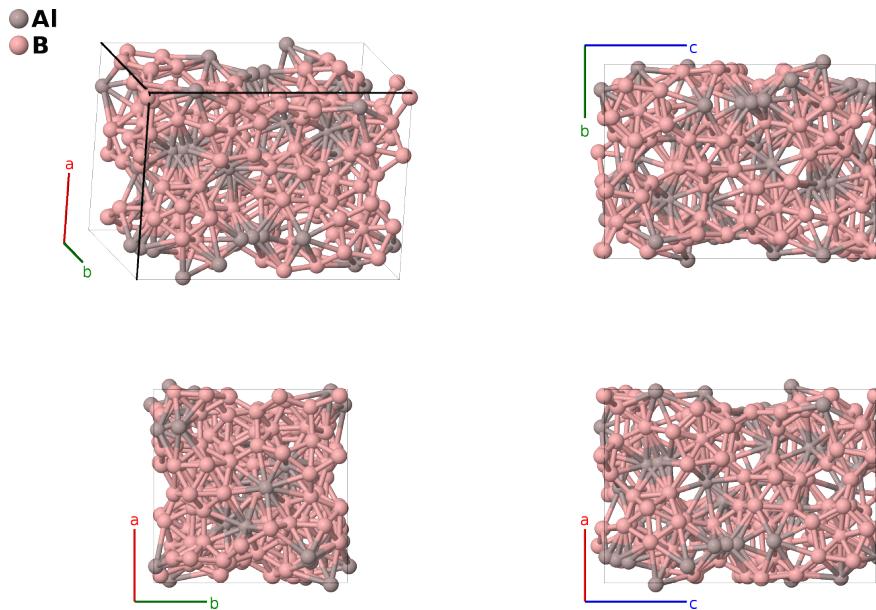


α -AlB₁₂ Structure: A5B22_tP216_96_5b_2a21b-001

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<https://aflow.org/p/ZF6C>

https://aflow.org/p/A5B22_tP216_96_5b_2a21b-001



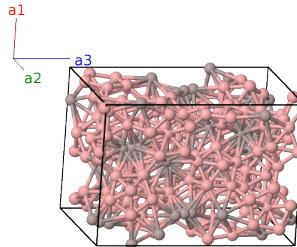
Prototype	AlB ₁₂
AFLOW prototype label	A5B22_tP216_96_5b_2a21b-001
ICSD	1091
Pearson symbol	tP216
Space group number	96
Space group symbol	$P4_32_12$
AFLOW prototype command	<pre>aflow --proto=A5B22_tP216_96_5b_2a21b-001 --params=a,c/a,x1,x2,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6,x7,y7,z7,x8,y8,z8,x9, y9,z9,x10,y10,z10,x11,y11,z11,x12,y12,z12,x13,y13,z13,x14,y14,z14,x15,y15,z15,x16,y16,z16, x17,y17,z17,x18,y18,z18,x19,y19,z19,x20,y20,z20,x21,y21,z21,x22,y22,z22,x23,y23,z23,x24, y24,z24,x25,y25,z25,x26,y26,z26,x27,y27,z27,x28,y28,z28</pre>

- AlB₁₂ can also be found as orthorhombic γ -AlB₁₂. Unfortunately we do not have a determination of the atomic positions in that system.
- As the γ structure has never been isolated from the α structure, and can be transformed into the α structure but not reconstituted from it, α -AlB₁₂ is the ground state of the system. (Higashi, 2000)

- According to (Higashi, 1977), there are thirteen aluminum atoms in this cell, distributed statistically among the five sites. This gives a stoichiometry of $\text{Al}_{0.88}\text{B}_{12}$. The sites Al-I, Al-III, and Al-V are extremely close together. The combined site is 98% occupied, and only one site is occupied at any one position, so the occupancy of these sites are approximately 33%. Similarly, pairs of Al-II atoms are rather close together, and each pair of sites contains approximately 98%, giving an occupation of 49% for the A-II site. If there are thirteen aluminum atoms in the unit cell, puts the occupation of the Al-IV site at 14.5%.
- This structure can also be found in the enantiomorphic space group $P4_12_12$ #92. We follow the authors and place it in $P4_32_12$ #96.

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	$a x_1 \hat{\mathbf{x}} + a x_1 \hat{\mathbf{y}}$	(4a)	B I
\mathbf{B}_2	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$-a x_1 \hat{\mathbf{x}} - a x_1 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4a)	B I
\mathbf{B}_3	$-(x_1 - \frac{1}{2}) \mathbf{a}_1 + (x_1 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4a)	B I
\mathbf{B}_4	$(x_1 + \frac{1}{2}) \mathbf{a}_1 - (x_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4a)	B I
\mathbf{B}_5	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$a x_2 \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}}$	(4a)	B II
\mathbf{B}_6	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$-a x_2 \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4a)	B II
\mathbf{B}_7	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4a)	B II
\mathbf{B}_8	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4a)	B II
\mathbf{B}_9	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$a x_3 \hat{\mathbf{x}} + a y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(8b)	Al I
\mathbf{B}_{10}	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$-a x_3 \hat{\mathbf{x}} - a y_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Al I
\mathbf{B}_{11}	$-(y_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{3}{4}) \mathbf{a}_3$	$-a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	Al I
\mathbf{B}_{12}	$(y_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{4}) \mathbf{a}_3$	$a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Al I
\mathbf{B}_{13}	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{3}{4}) \mathbf{a}_3$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	Al I
\mathbf{B}_{14}	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{4}) \mathbf{a}_3$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Al I
\mathbf{B}_{15}	$y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$a y_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(8b)	Al I
\mathbf{B}_{16}	$-y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$-a y_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Al I
\mathbf{B}_{17}	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$a x_4 \hat{\mathbf{x}} + a y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(8b)	Al II
\mathbf{B}_{18}	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$-a x_4 \hat{\mathbf{x}} - a y_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Al II

B₄₈	$-y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	=	$-ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	A I V
B₄₉	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8b)	B III
B₅₀	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	=	$-ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	B III
B₅₁	$-(y_8 - \frac{1}{2}) \mathbf{a}_1 + (x_8 + \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{3}{4}) \mathbf{a}_3$	=	$-a(y_8 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_8 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	B III
B₅₂	$(y_8 + \frac{1}{2}) \mathbf{a}_1 - (x_8 - \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{4}) \mathbf{a}_3$	=	$a(y_8 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_8 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	B III
B₅₃	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{3}{4}) \mathbf{a}_3$	=	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	B III
B₅₄	$(x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{4}) \mathbf{a}_3$	=	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_8 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	B III
B₅₅	$y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	=	$ay_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8b)	B III
B₅₆	$-y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	=	$-ay_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	B III
B₅₇	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$ax_9 \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8b)	B IV
B₅₈	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	=	$-ax_9 \hat{\mathbf{x}} - ay_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	B IV
B₅₉	$-(y_9 - \frac{1}{2}) \mathbf{a}_1 + (x_9 + \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{3}{4}) \mathbf{a}_3$	=	$-a(y_9 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_9 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_9 + \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	B IV
B₆₀	$(y_9 + \frac{1}{2}) \mathbf{a}_1 - (x_9 - \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{4}) \mathbf{a}_3$	=	$a(y_9 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_9 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	B IV
B₆₁	$-(x_9 - \frac{1}{2}) \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - (z_9 - \frac{3}{4}) \mathbf{a}_3$	=	$-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	B IV
B₆₂	$(x_9 + \frac{1}{2}) \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 - (z_9 - \frac{1}{4}) \mathbf{a}_3$	=	$a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_9 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	B IV
B₆₃	$y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	=	$ay_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8b)	B IV
B₆₄	$-y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$	=	$-ay_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	B IV
B₆₅	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	=	$ax_{10} \hat{\mathbf{x}} + ay_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8b)	B V
B₆₆	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	=	$-ax_{10} \hat{\mathbf{x}} - ay_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	B V
B₆₇	$-(y_{10} - \frac{1}{2}) \mathbf{a}_1 + (x_{10} + \frac{1}{2}) \mathbf{a}_2 + (z_{10} + \frac{3}{4}) \mathbf{a}_3$	=	$-a(y_{10} - \frac{1}{2}) \hat{\mathbf{x}} + a(x_{10} + \frac{1}{2}) \hat{\mathbf{y}} + c(z_{10} + \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	B V
B₆₈	$(y_{10} + \frac{1}{2}) \mathbf{a}_1 - (x_{10} - \frac{1}{2}) \mathbf{a}_2 + (z_{10} + \frac{1}{4}) \mathbf{a}_3$	=	$a(y_{10} + \frac{1}{2}) \hat{\mathbf{x}} - a(x_{10} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{10} + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	B V
B₆₉	$-(x_{10} - \frac{1}{2}) \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 - (z_{10} - \frac{3}{4}) \mathbf{a}_3$	=	$-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} + a(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{10} - \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	B V
B₇₀	$(x_{10} + \frac{1}{2}) \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 - (z_{10} - \frac{1}{4}) \mathbf{a}_3$	=	$a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} - a(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} - c(z_{10} - \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	B V
B₇₁	$y_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	=	$ay_{10} \hat{\mathbf{x}} + ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8b)	B V
B₇₂	$-y_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3$	=	$-ay_{10} \hat{\mathbf{x}} - ax_{10} \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	B V
B₇₃	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	=	$ax_{11} \hat{\mathbf{x}} + ay_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(8b)	B VI
B₇₄	$-x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3$	=	$-ax_{11} \hat{\mathbf{x}} - ay_{11} \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	B VI
B₇₅	$-(y_{11} - \frac{1}{2}) \mathbf{a}_1 + (x_{11} + \frac{1}{2}) \mathbf{a}_2 + (z_{11} + \frac{3}{4}) \mathbf{a}_3$	=	$-a(y_{11} - \frac{1}{2}) \hat{\mathbf{x}} + a(x_{11} + \frac{1}{2}) \hat{\mathbf{y}} + c(z_{11} + \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	B VI
B₇₆	$(y_{11} + \frac{1}{2}) \mathbf{a}_1 - (x_{11} - \frac{1}{2}) \mathbf{a}_2 + (z_{11} + \frac{1}{4}) \mathbf{a}_3$	=	$a(y_{11} + \frac{1}{2}) \hat{\mathbf{x}} - a(x_{11} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{11} + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	B VI
B₇₇	$-(x_{11} - \frac{1}{2}) \mathbf{a}_1 + (y_{11} + \frac{1}{2}) \mathbf{a}_2 - (z_{11} - \frac{3}{4}) \mathbf{a}_3$	=	$-a(x_{11} - \frac{1}{2}) \hat{\mathbf{x}} + a(y_{11} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{11} - \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	B VI

$\mathbf{B}_{197} =$	$-\left(x_{26} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{26} + \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(z_{26} - \frac{3}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_{26} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_{26} + \frac{1}{2}\right) \hat{\mathbf{y}} -$ $c\left(z_{26} - \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	B XXI
$\mathbf{B}_{198} =$	$\left(x_{26} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{26} - \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(z_{26} - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_{26} + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_{26} - \frac{1}{2}\right) \hat{\mathbf{y}} -$ $c\left(z_{26} - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	B XXI
$\mathbf{B}_{199} =$	$y_{26} \mathbf{a}_1 + x_{26} \mathbf{a}_2 - z_{26} \mathbf{a}_3$	$=$	$ay_{26} \hat{\mathbf{x}} + ax_{26} \hat{\mathbf{y}} - cz_{26} \hat{\mathbf{z}}$	(8b)	B XXI
$\mathbf{B}_{200} =$	$-y_{26} \mathbf{a}_1 - x_{26} \mathbf{a}_2 - \left(z_{26} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_{26} \hat{\mathbf{x}} - ax_{26} \hat{\mathbf{y}} - c\left(z_{26} - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	B XXI
$\mathbf{B}_{201} =$	$x_{27} \mathbf{a}_1 + y_{27} \mathbf{a}_2 + z_{27} \mathbf{a}_3$	$=$	$ax_{27} \hat{\mathbf{x}} + ay_{27} \hat{\mathbf{y}} + cz_{27} \hat{\mathbf{z}}$	(8b)	B XXII
$\mathbf{B}_{202} =$	$-x_{27} \mathbf{a}_1 - y_{27} \mathbf{a}_2 + \left(z_{27} + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_{27} \hat{\mathbf{x}} - ay_{27} \hat{\mathbf{y}} + c\left(z_{27} + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	B XXII
$\mathbf{B}_{203} =$	$-\left(y_{27} - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_{27} + \frac{1}{2}\right) \mathbf{a}_2 +$ $\left(z_{27} + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$-a\left(y_{27} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_{27} + \frac{1}{2}\right) \hat{\mathbf{y}} +$ $c\left(z_{27} + \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	B XXII
$\mathbf{B}_{204} =$	$\left(y_{27} + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{27} - \frac{1}{2}\right) \mathbf{a}_2 +$ $\left(z_{27} + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$a\left(y_{27} + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_{27} - \frac{1}{2}\right) \hat{\mathbf{y}} +$ $c\left(z_{27} + \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	B XXII
$\mathbf{B}_{205} =$	$-\left(x_{27} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{27} + \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(z_{27} - \frac{3}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_{27} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_{27} + \frac{1}{2}\right) \hat{\mathbf{y}} -$ $c\left(z_{27} - \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	B XXII
$\mathbf{B}_{206} =$	$\left(x_{27} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{27} - \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(z_{27} - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_{27} + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_{27} - \frac{1}{2}\right) \hat{\mathbf{y}} -$ $c\left(z_{27} - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	B XXII
$\mathbf{B}_{207} =$	$y_{27} \mathbf{a}_1 + x_{27} \mathbf{a}_2 - z_{27} \mathbf{a}_3$	$=$	$ay_{27} \hat{\mathbf{x}} + ax_{27} \hat{\mathbf{y}} - cz_{27} \hat{\mathbf{z}}$	(8b)	B XXII
$\mathbf{B}_{208} =$	$-y_{27} \mathbf{a}_1 - x_{27} \mathbf{a}_2 - \left(z_{27} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_{27} \hat{\mathbf{x}} - ax_{27} \hat{\mathbf{y}} - c\left(z_{27} - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	B XXII
$\mathbf{B}_{209} =$	$x_{28} \mathbf{a}_1 + y_{28} \mathbf{a}_2 + z_{28} \mathbf{a}_3$	$=$	$ax_{28} \hat{\mathbf{x}} + ay_{28} \hat{\mathbf{y}} + cz_{28} \hat{\mathbf{z}}$	(8b)	B XXIII
$\mathbf{B}_{210} =$	$-x_{28} \mathbf{a}_1 - y_{28} \mathbf{a}_2 + \left(z_{28} + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_{28} \hat{\mathbf{x}} - ay_{28} \hat{\mathbf{y}} + c\left(z_{28} + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	B XXIII
$\mathbf{B}_{211} =$	$-\left(y_{28} - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_{28} + \frac{1}{2}\right) \mathbf{a}_2 +$ $\left(z_{28} + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$-a\left(y_{28} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_{28} + \frac{1}{2}\right) \hat{\mathbf{y}} +$ $c\left(z_{28} + \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	B XXIII
$\mathbf{B}_{212} =$	$\left(y_{28} + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{28} - \frac{1}{2}\right) \mathbf{a}_2 +$ $\left(z_{28} + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$a\left(y_{28} + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_{28} - \frac{1}{2}\right) \hat{\mathbf{y}} +$ $c\left(z_{28} + \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	B XXIII
$\mathbf{B}_{213} =$	$-\left(x_{28} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{28} + \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(z_{28} - \frac{3}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_{28} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_{28} + \frac{1}{2}\right) \hat{\mathbf{y}} -$ $c\left(z_{28} - \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	B XXIII
$\mathbf{B}_{214} =$	$\left(x_{28} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{28} - \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(z_{28} - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_{28} + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_{28} - \frac{1}{2}\right) \hat{\mathbf{y}} -$ $c\left(z_{28} - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	B XXIII
$\mathbf{B}_{215} =$	$y_{28} \mathbf{a}_1 + x_{28} \mathbf{a}_2 - z_{28} \mathbf{a}_3$	$=$	$ay_{28} \hat{\mathbf{x}} + ax_{28} \hat{\mathbf{y}} - cz_{28} \hat{\mathbf{z}}$	(8b)	B XXIII
$\mathbf{B}_{216} =$	$-y_{28} \mathbf{a}_1 - x_{28} \mathbf{a}_2 - \left(z_{28} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_{28} \hat{\mathbf{x}} - ax_{28} \hat{\mathbf{y}} - c\left(z_{28} - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	B XXIII

References

- [1] I. Higashi, T. Sakurai, and T. Atoda, *Crystal Structure of α -AlB₁₂*, J. Solid State Chem. **20**, 67–77 (1977), doi:10.1016/0022-4596(77)90052-4.
- [2] I. Higashi, *Crystal Chemistry of α -AlB₁₂ and γ -AlB₁₂*, J. Solid State Chem. **154**, 168–176 (2000), doi:10.1006/jssc.2000.8831.