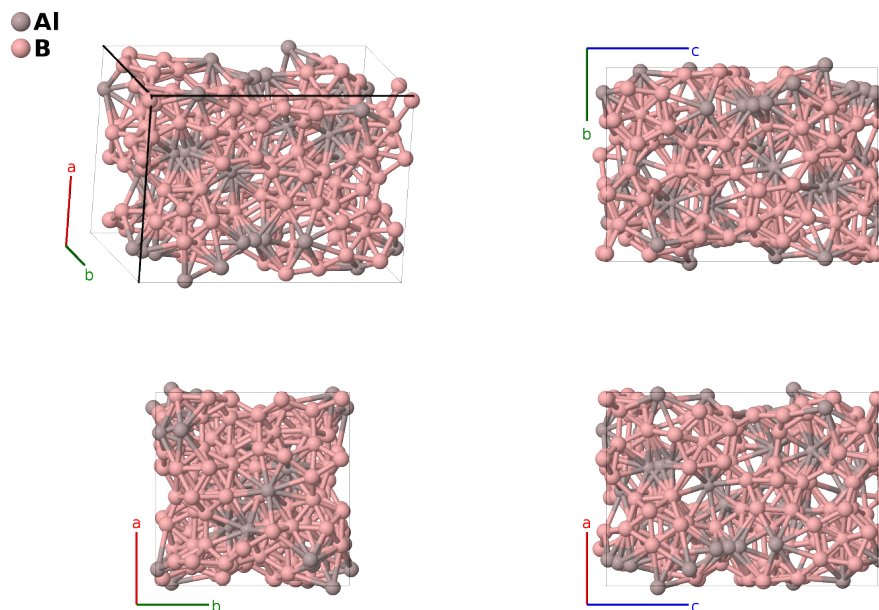


# $\alpha$ -AlB<sub>12</sub> Structure: A5B22\_tP216\_96\_5b\_2a21b-001

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

[https://afLOW.org/p/A5B22\\_tP216\\_96\\_5b\\_2a21b-001](https://afLOW.org/p/A5B22_tP216_96_5b_2a21b-001)



Prototype	AlB <sub>12</sub>
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>

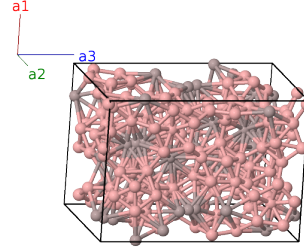
- AlB<sub>12</sub> can also be found as orthorhombic  $\gamma$ -AlB<sub>12</sub>. Unfortunately we do not have a determination of the atomic positions in that system.
- As the  $\gamma$  structure has never been isolated from the  $\alpha$  structure, and can be transformed into the  $\alpha$  structure but not reconstituted from it,  $\alpha$ -AlB<sub>12</sub> 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.

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### Simple Tetragonal primitive vectors

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




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### 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















$$\begin{aligned}
\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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{B XXIII}
\end{aligned}$$

## References

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