$MgAlB_{14}$ Structure: AB14C2_oI68_74_a_3i2j_h-001

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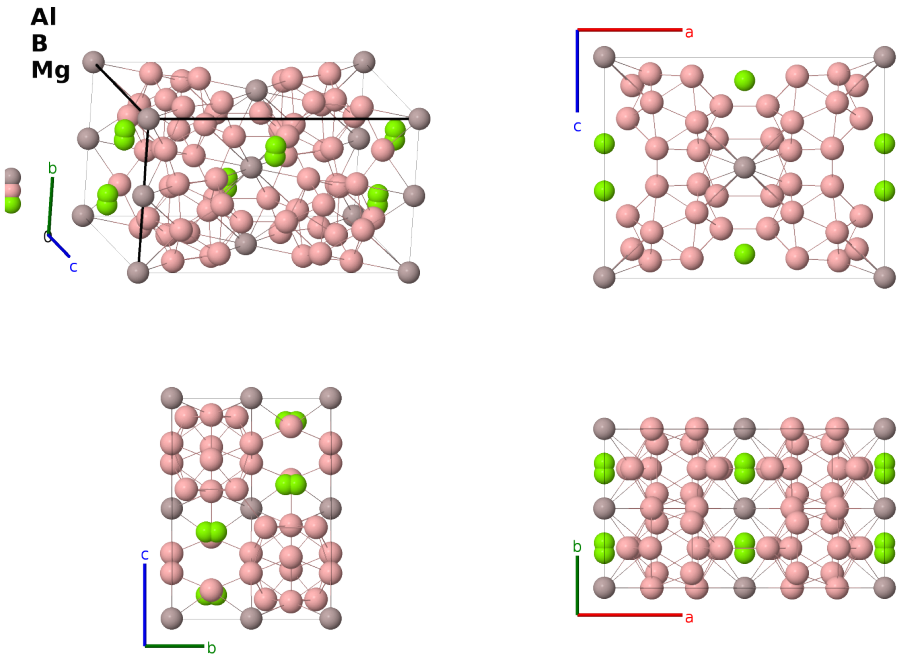
https://aflow.org/prototype-encyclopedia/U35P

https://aflow.org/prototype-encyclopedia/AB14C2_oI68_74_a_3i2j_h-001



Prototype	$AlB_{14}Mg$
AFLOW prototype label	AB14C2_oI68_74_a_3i2j_h-001
ICSD	30728
CCDC	1604969
Pearson symbol	oI68
Space group number	74
Space group symbol	*Imma*
AFLOW prototype command	`aflow --proto=AB14C2_oI68_74_a_3i2j_h-001 --params=`$a, b/a, c/a, y_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

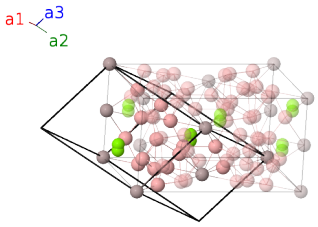
Other compounds with this structure

$DyAlB_{14}$, $ErAlB_{14}$, $HoAlB_{14}$, $LiAlB_{14}$, $LuAlB_{14}$, $ScAlB_{14}$, $TbAlB_{14}$, $TmAlB_{14}$, $YbAlB_{14}$

- The Al (4a) sites are only occupied 74.8% of the time, and the Mg (8h) sites is only occupied 39.0% of the time, so the the actual composition of this sample is $Mg_{0.780}Al_{0.748}B_{14}$.
- The atoms on the Mg (8h) site form pairs separated by 0.4Å, much too close to be physical, so at most only one site in each pair can be occupied. Alternatively, if we set $y_2 = 3/4$ for the Mg I atom then the pairs merge to become a (4e) site, with occupation 0.78, making this equivalent to our $NaAlB_{14}$ structure. This structure may be more convenient for electronic structure calculations.
- (Higashi, 1983) give the structure in the *Imam* setting of space group #74. We used FINDSYM and AFLOW to transform this to the standard *Imma* setting.

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
$\mathbf{B_1}$	=	0	=	0	(4a)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}}$	(4a)	Al I
$\mathbf{B_3}$	=	$(y_2 + z_2)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8h)	Mg I
$\mathbf{B_4}$	=	$\left(-y_2 + z_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8h)	Mg I
$\mathbf{B_5}$	=	$\left(y_2 - z_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8h)	Mg I
$\mathbf{B_6}$	=	$-(y_2 + z_2)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8h)	Mg I
$\mathbf{B_7}$	=	$\left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + \left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8i)	B I
$\mathbf{B_8}$	=	$\left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8i)	B I
$\mathbf{B_9}$	=	$-\left(z_3 - \frac{3}{4}\right)\,\mathbf{a}_1 - (x_3 + z_3)\,\mathbf{a}_2 - \left(x_3 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8i)	B I
$\mathbf{B_{10}}$	=	$-\left(z_3 - \frac{3}{4}\right)\,\mathbf{a}_1 + (x_3 - z_3)\,\mathbf{a}_2 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8i)	B I
$\mathbf{B_{11}}$	=	$\left(z_4 + \frac{1}{4}\right)\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + \left(x_4 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8i)	B II
$\mathbf{B_{12}}$	=	$\left(z_4 + \frac{1}{4}\right)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - \left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8i)	B II
$\mathbf{B_{13}}$	=	$-\left(z_4 - \frac{3}{4}\right)\,\mathbf{a}_1 - (x_4 + z_4)\,\mathbf{a}_2 - \left(x_4 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8i)	B II
$\mathbf{B_{14}}$	=	$-\left(z_4 - \frac{3}{4}\right)\,\mathbf{a}_1 + (x_4 - z_4)\,\mathbf{a}_2 + \left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8i)	B II

$$\mathbf{B_{15}} = \left(z_5+\tfrac{1}{4}\right)\mathbf{a}_1+(x_5+z_5)\,\mathbf{a}_2+\left(x_5+\tfrac{1}{4}\right)\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}}+\tfrac{1}{4}b\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}} \quad (8i) \quad \text{B III}$$

$$\mathbf{B_{16}} = \left(z_5+\tfrac{1}{4}\right)\mathbf{a}_1-(x_5-z_5)\,\mathbf{a}_2-\left(x_5-\tfrac{1}{4}\right)\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}}+\tfrac{1}{4}b\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}} \quad (8i) \quad \text{B III}$$

$$\mathbf{B_{17}} = -\left(z_5-\tfrac{3}{4}\right)\mathbf{a}_1-(x_5+z_5)\,\mathbf{a}_2-\left(x_5-\tfrac{3}{4}\right)\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}}+\tfrac{3}{4}b\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}} \quad (8i) \quad \text{B III}$$

$$\mathbf{B_{18}} = -\left(z_5-\tfrac{3}{4}\right)\mathbf{a}_1+(x_5-z_5)\,\mathbf{a}_2+\left(x_5+\tfrac{3}{4}\right)\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}}+\tfrac{3}{4}b\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}} \quad (8i) \quad \text{B III}$$

$$\mathbf{B_{19}} = (y_6+z_6)\,\mathbf{a}_1+(x_6+z_6)\,\mathbf{a}_2+(x_6+y_6)\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}}+by_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}} \quad (16j) \quad \text{B IV}$$

$$\mathbf{B_{20}} = \left(-y_6+z_6+\tfrac{1}{2}\right)\mathbf{a}_1-(x_6-z_6)\,\mathbf{a}_2-\left(x_6+y_6-\tfrac{1}{2}\right)\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}}-b\left(y_6-\tfrac{1}{2}\right)\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}} \quad (16j) \quad \text{B IV}$$

$$\mathbf{B_{21}} = \left(y_6-z_6+\tfrac{1}{2}\right)\mathbf{a}_1-(x_6+z_6)\,\mathbf{a}_2+\left(-x_6+y_6+\tfrac{1}{2}\right)\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}}+b\left(y_6+\tfrac{1}{2}\right)\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}} \quad (16j) \quad \text{B IV}$$

$$\mathbf{B_{22}} = -(y_6+z_6)\,\mathbf{a}_1+(x_6-z_6)\,\mathbf{a}_2+(x_6-y_6)\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}}-by_6\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}} \quad (16j) \quad \text{B IV}$$

$$\mathbf{B_{23}} = -(y_6+z_6)\,\mathbf{a}_1-(x_6+z_6)\,\mathbf{a}_2-(x_6+y_6)\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}}-by_6\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}} \quad (16j) \quad \text{B IV}$$

$$\mathbf{B_{24}} = \left(y_6-z_6+\tfrac{1}{2}\right)\mathbf{a}_1+(x_6-z_6)\,\mathbf{a}_2+\left(x_6+y_6+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}}+b\left(y_6+\tfrac{1}{2}\right)\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}} \quad (16j) \quad \text{B IV}$$

$$\mathbf{B_{25}} = \left(-y_6+z_6+\tfrac{1}{2}\right)\mathbf{a}_1+(x_6+z_6)\,\mathbf{a}_2+\left(x_6-y_6+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}}-b\left(y_6-\tfrac{1}{2}\right)\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}} \quad (16j) \quad \text{B IV}$$

$$\mathbf{B_{26}} = (y_6+z_6)\,\mathbf{a}_1-(x_6-z_6)\,\mathbf{a}_2-(x_6-y_6)\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}}+by_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}} \quad (16j) \quad \text{B IV}$$

$$\mathbf{B_{27}} = (y_7+z_7)\,\mathbf{a}_1+(x_7+z_7)\,\mathbf{a}_2+(x_7+y_7)\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{B V}$$

$$\mathbf{B_{28}} = \left(-y_7+z_7+\tfrac{1}{2}\right)\mathbf{a}_1-(x_7-z_7)\,\mathbf{a}_2-\left(x_7+y_7-\tfrac{1}{2}\right)\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}}-b\left(y_7-\tfrac{1}{2}\right)\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{B V}$$

$$\mathbf{B_{29}} = \left(y_7-z_7+\tfrac{1}{2}\right)\mathbf{a}_1-(x_7+z_7)\,\mathbf{a}_2+\left(-x_7+y_7+\tfrac{1}{2}\right)\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}}+b\left(y_7+\tfrac{1}{2}\right)\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{B V}$$

$$\mathbf{B_{30}} = -(y_7+z_7)\,\mathbf{a}_1+(x_7-z_7)\,\mathbf{a}_2+(x_7-y_7)\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{B V}$$

$$\mathbf{B_{31}} = -(y_7+z_7)\,\mathbf{a}_1-(x_7+z_7)\,\mathbf{a}_2-(x_7+y_7)\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{B V}$$

$$\mathbf{B_{32}} = \left(y_7-z_7+\tfrac{1}{2}\right)\mathbf{a}_1+(x_7-z_7)\,\mathbf{a}_2+\left(x_7+y_7+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}}+b\left(y_7+\tfrac{1}{2}\right)\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{B V}$$

$$\mathbf{B_{33}} = \left(-y_7+z_7+\tfrac{1}{2}\right)\mathbf{a}_1+(x_7+z_7)\,\mathbf{a}_2+\left(x_7-y_7+\tfrac{1}{2}\right)\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}}-b\left(y_7-\tfrac{1}{2}\right)\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{B V}$$

$$\mathbf{B_{34}} = (y_7+z_7)\,\mathbf{a}_1-(x_7-z_7)\,\mathbf{a}_2-(x_7-y_7)\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} \quad (16j) \quad \text{B V}$$

References

[1] I. Higashi and T. Ito, *Refinement of the Structure of $MgAlB_{14}$*, J. Less-Common Met. **92**, 239–246 (1983), doi:10.1016/0022-5088(83)90490-3.

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