$Mg_{17}Al_{12}$ Structure: A12B17_cI58_217_g_acg-001

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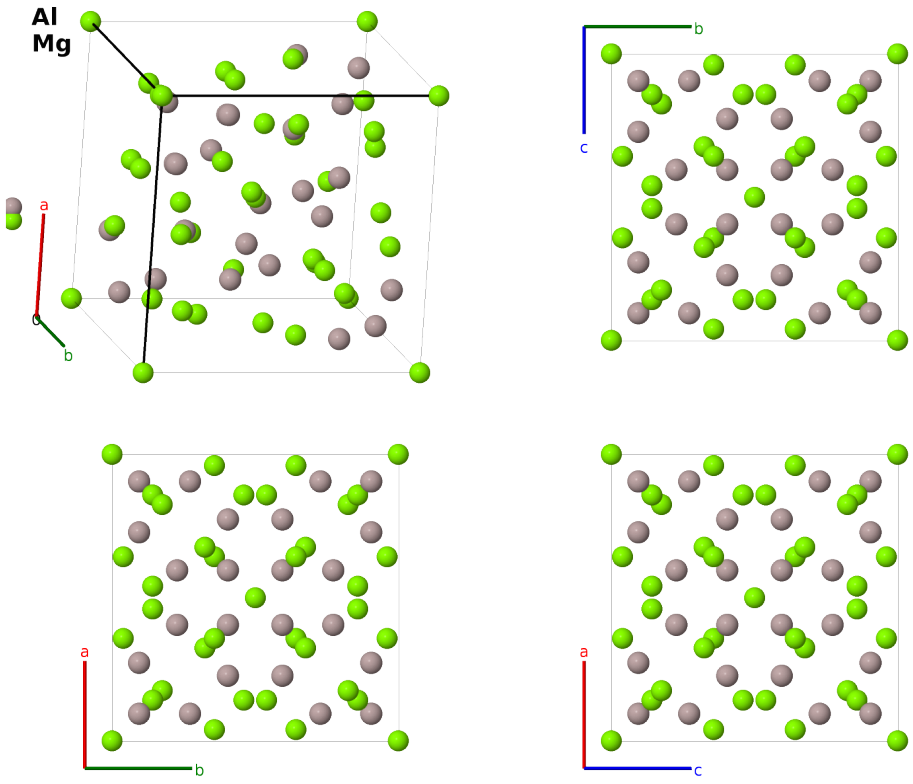
https://aflow.org/prototype-encyclopedia/56N2

https://aflow.org/prototype-encyclopedia/A12B17_cI58_217_g_acg-001

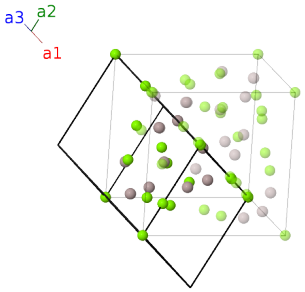


Prototype	$Al_{12}Mg_{17}$
AFLOW prototype label	A12B17_cI58_217_g_acg-001
ICSD	23607
CCDC	1599709
Pearson symbol	cI58
Space group number	217
Space group symbol	$I\bar{4}3m$
AFLOW prototype command	`aflow --proto=A12B17_cI58_217_g_acg-001 --params=`$a, x_2, x_3, z_3, x_4, z_4$

- This is a binary form of α-Mn ($A12$).

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Mg I
$\mathbf{B_2}$	=	$2x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + 2x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	Mg II
$\mathbf{B_3}$	=	$-2x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	Mg II
$\mathbf{B_4}$	=	$-2x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	Mg II
$\mathbf{B_5}$	=	$-2x_2\,\mathbf{a}_1$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	Mg II
$\mathbf{B_6}$	=	$(x_3 + z_3)\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + 2x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_7}$	=	$-(x_3 - z_3)\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - 2x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_8}$	=	$(x_3 - z_3)\,\mathbf{a}_1 - (x_3 + z_3)\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_9}$	=	$-(x_3 + z_3)\,\mathbf{a}_1 + (x_3 - z_3)\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_{10}}$	=	$2x_3\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + (x_3 + z_3)\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_{11}}$	=	$-2x_3\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - (x_3 - z_3)\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_{12}}$	=	$(x_3 - z_3)\,\mathbf{a}_2 - (x_3 + z_3)\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_{13}}$	=	$-(x_3 + z_3)\,\mathbf{a}_2 + (x_3 - z_3)\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_{14}}$	=	$(x_3 + z_3)\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2 + (x_3 + z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_{15}}$	=	$-(x_3 - z_3)\,\mathbf{a}_1 - 2x_3\,\mathbf{a}_2 - (x_3 - z_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_{16}}$	=	$-(x_3 + z_3)\,\mathbf{a}_1 + (x_3 - z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_{17}}$	=	$(x_3 - z_3)\,\mathbf{a}_1 - (x_3 + z_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(24g)	Al I
$\mathbf{B_{18}}$	=	$(x_4 + z_4)\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + 2x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(24g)	Mg III
$\mathbf{B_{19}}$	=	$-(x_4 - z_4)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - 2x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(24g)	Mg III
$\mathbf{B_{20}}$	=	$(x_4 - z_4)\,\mathbf{a}_1 - (x_4 + z_4)\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}}$	(24g)	Mg III
$\mathbf{B_{21}}$	=	$-(x_4 + z_4)\,\mathbf{a}_1 + (x_4 - z_4)\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}}$	(24g)	Mg III

$\mathbf{B_{22}}$	=	$2x_4\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + (x_4 + z_4)\,\mathbf{a}_3$	=	$az_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(24g)	Mg III
$\mathbf{B_{23}}$	=	$-2x_4\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - (x_4 - z_4)\,\mathbf{a}_3$	=	$az_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(24g)	Mg III
$\mathbf{B_{24}}$	=	$(x_4 - z_4)\,\mathbf{a}_2 - (x_4 + z_4)\,\mathbf{a}_3$	=	$-az_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(24g)	Mg III
$\mathbf{B_{25}}$	=	$-(x_4 + z_4)\,\mathbf{a}_2 + (x_4 - z_4)\,\mathbf{a}_3$	=	$-az_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(24g)	Mg III
$\mathbf{B_{26}}$	=	$(x_4 + z_4)\,\mathbf{a}_1 + 2x_4\,\mathbf{a}_2 + (x_4 + z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(24g)	Mg III
$\mathbf{B_{27}}$	=	$-(x_4 - z_4)\,\mathbf{a}_1 - 2x_4\,\mathbf{a}_2 - (x_4 - z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(24g)	Mg III
$\mathbf{B_{28}}$	=	$-(x_4 + z_4)\,\mathbf{a}_1 + (x_4 - z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - az_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(24g)	Mg III
$\mathbf{B_{29}}$	=	$(x_4 - z_4)\,\mathbf{a}_1 - (x_4 + z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - az_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(24g)	Mg III

References

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First cited in

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