

Ca₄Al₃Mg Structure:

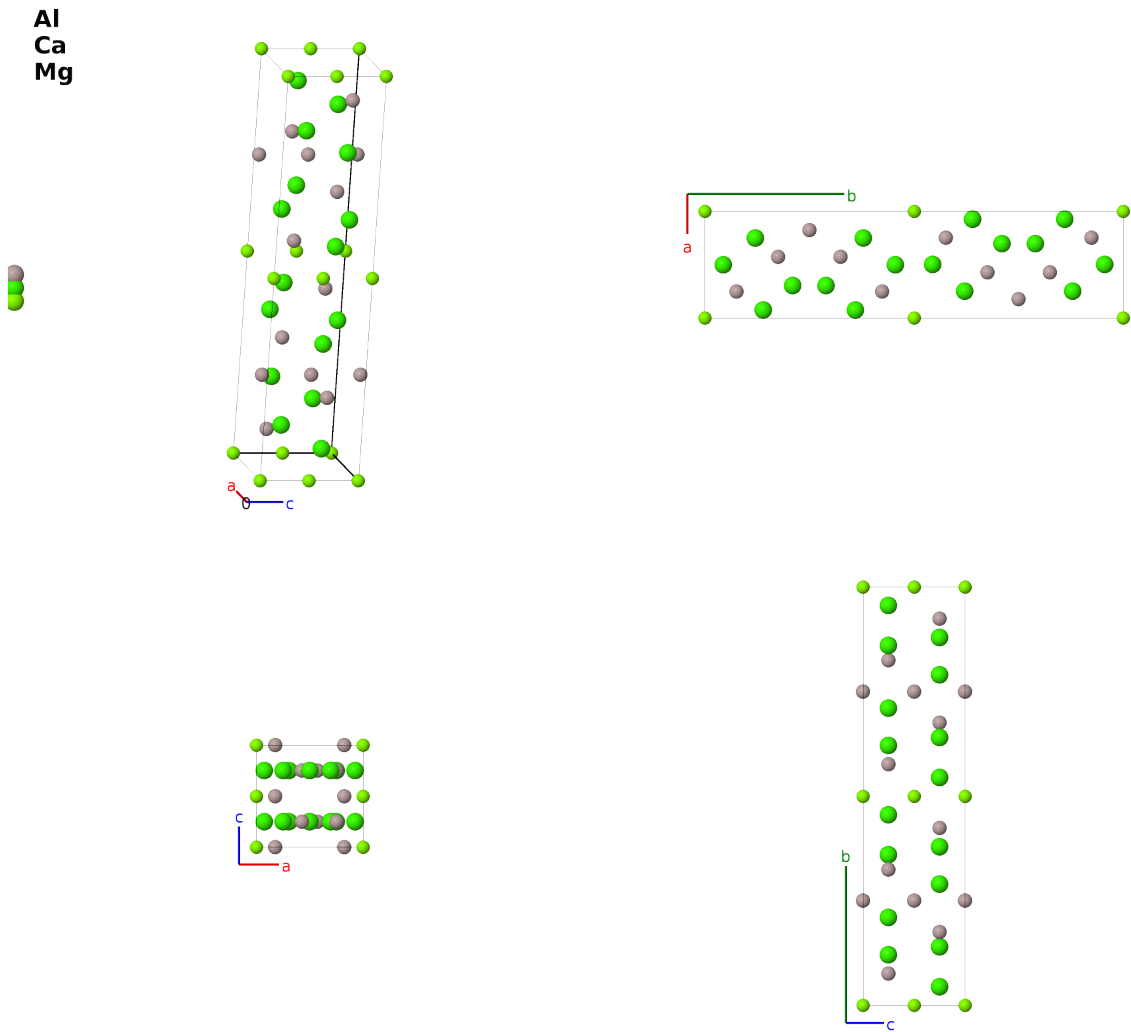
A3B4C_oP32_57_c2d_4d_a-001

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<https://aflow.org/prototype-encyclopedia/6529>

https://aflow.org/prototype-encyclopedia/A3B4C_oP32_57_c2d_4d_a-001



Prototype	Al ₃ Ca ₄ Mg
AFLOW prototype label	A3B4C_oP32_57_c2d_4d_a-001
ICSD	152756
CCDC	1669481
Pearson symbol	oP32

Space group number 57

Space group symbol *Pbcm*

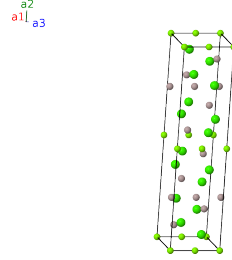
AFLOW prototype command `aflow --proto=A3B4C_oP32_57_c2d_4d_a-001`
`--params=a,b/a,c/a,x2,x3,y3,x4,y4,x5,y5,x6,y6,x7,y7,x8,y8`

Simple Orthorhombic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(4a)	Mg I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(4a)	Mg I
$\mathbf{B}_3$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4a)	Mg I
$\mathbf{B}_4$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} b \hat{\mathbf{y}}$	(4a)	Mg I
$\mathbf{B}_5$	$x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}}$	(4c)	Al I
$\mathbf{B}_6$	$-x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B}_7$	$-x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}}$	(4c)	Al I
$\mathbf{B}_8$	$x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4c)	Al I
$\mathbf{B}_9$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Al II
$\mathbf{B}_{10}$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	Al II
$\mathbf{B}_{11}$	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Al II
$\mathbf{B}_{12}$	$x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	Al II
$\mathbf{B}_{13}$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Al III
$\mathbf{B}_{14}$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	Al III
$\mathbf{B}_{15}$	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Al III
$\mathbf{B}_{16}$	$x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	Al III
$\mathbf{B}_{17}$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Ca I
$\mathbf{B}_{18}$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	Ca I
$\mathbf{B}_{19}$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Ca I
$\mathbf{B}_{20}$	$x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	Ca I
$\mathbf{B}_{21}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Ca II
$\mathbf{B}_{22}$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	Ca II
$\mathbf{B}_{23}$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Ca II

$\mathbf{B}_{24}$	$=$	$x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4d)	Ca II
$\mathbf{B}_{25}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	Ca III
$\mathbf{B}_{26}$	$=$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4d)	Ca III
$\mathbf{B}_{27}$	$=$	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	Ca III
$\mathbf{B}_{28}$	$=$	$x_7 \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4d)	Ca III
$\mathbf{B}_{29}$	$=$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	Ca IV
$\mathbf{B}_{30}$	$=$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4d)	Ca IV
$\mathbf{B}_{31}$	$=$	$-x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	Ca IV
$\mathbf{B}_{32}$	$=$	$x_8 \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4d)	Ca IV

References

- [1] Q. A. Zhang, W. M. Yang, and E. Akiba, *Synthesis and crystal structure of a new ternary compound $\text{Ca}_4\text{Al}_3\text{Mg}$* , J. Alloys Compd. **398**, 123–126 (2005), doi:10.1016/j.jallcom.2005.02.040.

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