

Ga₂Mg₅ ($D8_g$) Structure: A2B5_oI28_72_j_afj-001

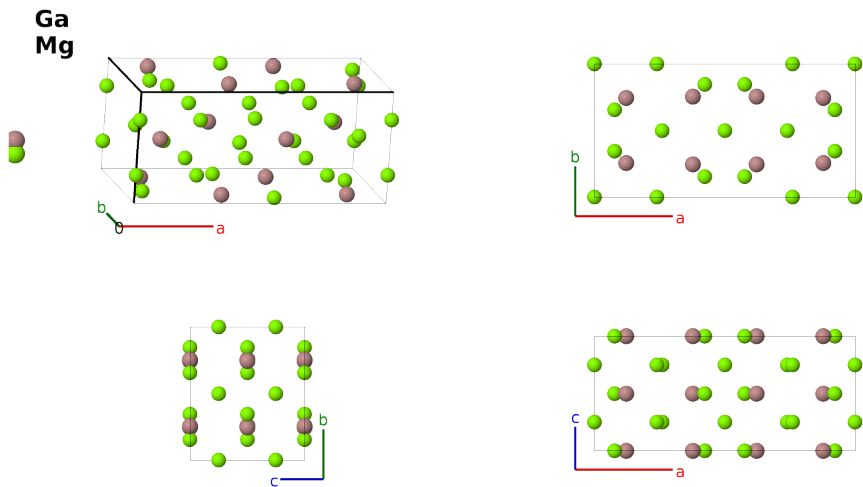
This structure previously used the label(s) **A2B5_oI28.72_j_bfj**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/AB10>

https://aflow.org/prototype-encyclopedia/A2B5_oI28_72_j_afj-001



Prototype	Ga ₂ Mg ₅
AFLOW prototype label	A2B5_oI28_72_j_afj-001
<i>Strukturbericht</i> designation	$D8_g$
ICSD	103794
CCDC	1661729
Pearson symbol	oI28
Space group number	72
Space group symbol	$Ibam$
AFLOW prototype command	<code>aflow --proto=A2B5_oI28_72_j_afj-001</code> <code>--params=a, b/a, c/a, x₂, x₃, y₃, x₄, y₄</code>

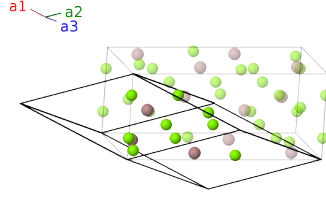
Other compounds with this structure

As₂Cu₅, In₂Mg₅, Tl₂Mg₅, Mn₂Ge₅

- We corrected an error in the Mg III (8j) coordinates and shifted the Mg I atoms from the (2b) to the (2a) site.

Body-centered Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(4a)	Mg I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(4a)	Mg I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + (x_2 + \frac{1}{4}) \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8f)	Mg II
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 - (x_2 - \frac{1}{4}) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8f)	Mg II
$\mathbf{B}_5$	$= \frac{3}{4} \mathbf{a}_1 - (x_2 - \frac{3}{4}) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8f)	Mg II
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 + (x_2 + \frac{3}{4}) \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8f)	Mg II
$\mathbf{B}_7$	$= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}}$	(8j)	Ga I
$\mathbf{B}_8$	$= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - (x_3 + y_3) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}}$	(8j)	Ga I
$\mathbf{B}_9$	$= (y_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8j)	Ga I
$\mathbf{B}_{10}$	$= -(y_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8j)	Ga I
$\mathbf{B}_{11}$	$= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}}$	(8j)	Mg III
$\mathbf{B}_{12}$	$= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - (x_4 + y_4) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}}$	(8j)	Mg III
$\mathbf{B}_{13}$	$= (y_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8j)	Mg III
$\mathbf{B}_{14}$	$= -(y_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8j)	Mg III

References

- [1] K. Schubert, K. Frank, R. Gohle, A. Maldonado, H. G. Meissner, A. Raman, and W. Rossteutscher, *Einige Strukturdaten metallischer Phasen (8)*, *Naturwissenschaften* **50**, 41 (1963), doi:10.1007/BF00622812.

Found in

- [1] V. Vreshch, *Crystallography online.com* (2018). Crystal Structure of Ga₂Mg₅.

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