

Mg₂Zn₁₁ (*D*8_c) Structure: A2B11_cP39_200_f_begik-001

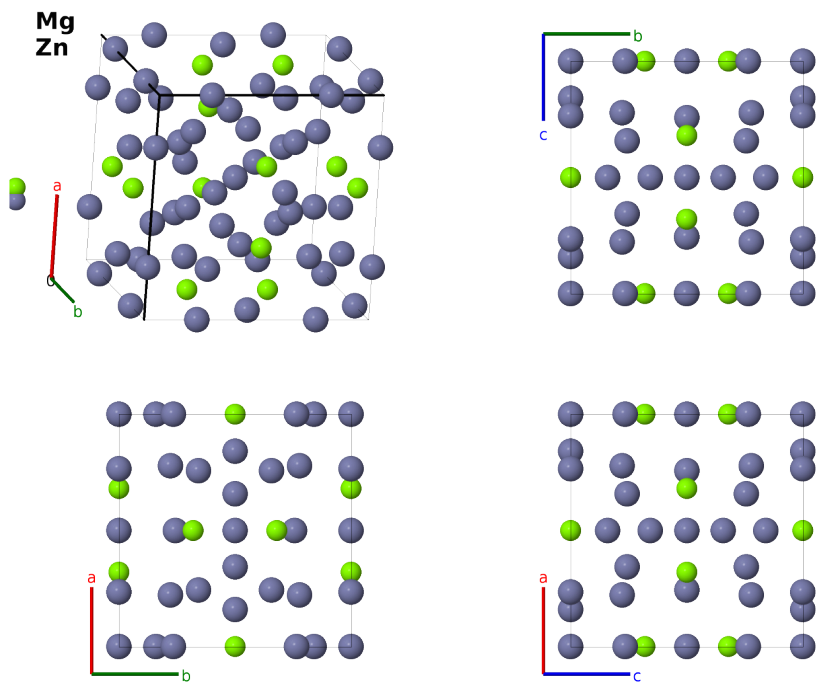
This structure previously used the label(s) **A2B11_cP39_200_f_aghi**j. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/8FHP>

https://aflow.org/prototype-encyclopedia/A2B11_cP39_200_f_begik-001



Prototype	Mg ₂ Zn ₁₁
AFLOW prototype label	A2B11_cP39_200_f_begik-001
<i>Strukturbericht</i> designation	<i>D</i> 8 _c
ICSD	104898
CCDC	1662799
Pearson symbol	cP39
Space group number	200
Space group symbol	<i>Pm</i> $\bar{3}$
AFLOW prototype command	<code>aflow --proto=A2B11_cP39_200_f_begik-001</code> <code>--params=<i>a</i>, <i>x</i>₂, <i>x</i>₃, <i>x</i>₄, <i>x</i>₅, <i>y</i>₆, <i>z</i>₆</code>

Other compounds with this structure

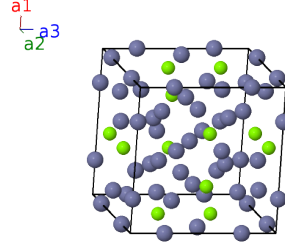
Na₂Cd₁₁, Mg₂Cu₆Al₅, Mg₂Cu₆Ga₅, Na₂Au₆In₅, Sc₂Co₇Ga₄, K₆Na₁₄CdTl₁₈, K₆Na₁₄HgTl₁₈, K₆Na₁₄MgTl₁₈, K₆Na₁₄ZnTl₁₈

Simple Cubic primitive vectors

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

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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
B ₁	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(1b)	Zn I
B ₂	$x_2 \mathbf{a}_1$	=	$ax_2 \hat{\mathbf{x}}$	(6e)	Zn II
B ₃	$-x_2 \mathbf{a}_1$	=	$-ax_2 \hat{\mathbf{x}}$	(6e)	Zn II
B ₄	$x_2 \mathbf{a}_2$	=	$ax_2 \hat{\mathbf{y}}$	(6e)	Zn II
B ₅	$-x_2 \mathbf{a}_2$	=	$-ax_2 \hat{\mathbf{y}}$	(6e)	Zn II
B ₆	$x_2 \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{z}}$	(6e)	Zn II
B ₇	$-x_2 \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{z}}$	(6e)	Zn II
B ₈	$x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f)	Mg I
B ₉	$-x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f)	Mg I
B ₁₀	$\frac{1}{2} \mathbf{a}_1 + x_3 \mathbf{a}_2$	=	$\frac{1}{2} a \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}}$	(6f)	Mg I
B ₁₁	$\frac{1}{2} \mathbf{a}_1 - x_3 \mathbf{a}_2$	=	$\frac{1}{2} a \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}}$	(6f)	Mg I
B ₁₂	$\frac{1}{2} \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(6f)	Mg I
B ₁₃	$\frac{1}{2} \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(6f)	Mg I
B ₁₄	$x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	=	$ax_4 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6g)	Zn III
B ₁₅	$-x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	=	$-ax_4 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6g)	Zn III
B ₁₆	$x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6g)	Zn III
B ₁₇	$-x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6g)	Zn III
B ₁₈	$\frac{1}{2} \mathbf{a}_1 + x_4 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + ax_4 \hat{\mathbf{z}}$	(6g)	Zn III
B ₁₉	$\frac{1}{2} \mathbf{a}_1 - x_4 \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} - ax_4 \hat{\mathbf{z}}$	(6g)	Zn III
B ₂₀	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(8i)	Zn IV
B ₂₁	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(8i)	Zn IV
B ₂₂	$-x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	=	$-ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(8i)	Zn IV
B ₂₃	$x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	=	$ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(8i)	Zn IV
B ₂₄	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	=	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(8i)	Zn IV
B ₂₅	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	=	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(8i)	Zn IV
B ₂₆	$x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(8i)	Zn IV

$\mathbf{B}_{27}$	$=$	$-x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(8i)	Zn IV
$\mathbf{B}_{28}$	$=$	$\frac{1}{2} \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}}$	(12k)	Zn V
$\mathbf{B}_{29}$	$=$	$\frac{1}{2} \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}}$	(12k)	Zn V
$\mathbf{B}_{30}$	$=$	$\frac{1}{2} \mathbf{a}_1 + y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}}$	(12k)	Zn V
$\mathbf{B}_{31}$	$=$	$\frac{1}{2} \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}}$	(12k)	Zn V
$\mathbf{B}_{32}$	$=$	$z_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$az_6 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}}$	(12k)	Zn V
$\mathbf{B}_{33}$	$=$	$z_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$az_6 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}}$	(12k)	Zn V
$\mathbf{B}_{34}$	$=$	$-z_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$-az_6 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}}$	(12k)	Zn V
$\mathbf{B}_{35}$	$=$	$-z_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$-az_6 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}}$	(12k)	Zn V
$\mathbf{B}_{36}$	$=$	$y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12k)	Zn V
$\mathbf{B}_{37}$	$=$	$-y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12k)	Zn V
$\mathbf{B}_{38}$	$=$	$y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12k)	Zn V
$\mathbf{B}_{39}$	$=$	$-y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12k)	Zn V

References

- [1] S. Samson, *Die Kristallstruktur von Mg_2Zn_{11}* , Acta Chem. Scand. **3**, 835–843 (1949), doi:10.3891/acta.chem.scand.03-0835.

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