

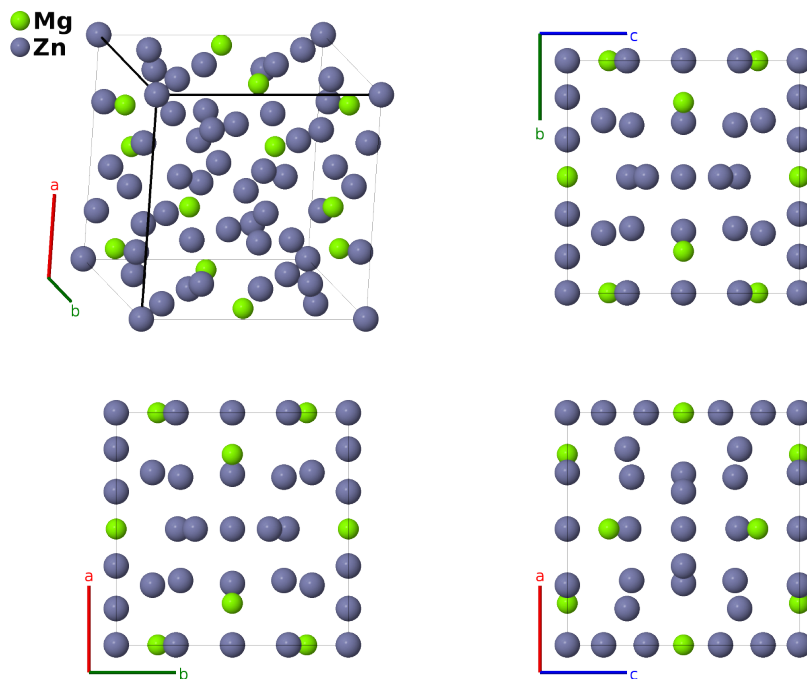
# Mg<sub>2</sub>Zn<sub>11</sub> ( $D8_c$ ) Structure: A2B11\_cP39\_200\_f\_begik-001

This structure originally had the label A2B11\_cP39\_200\_f\_aghij. Calls to that address will be redirected here.

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<https://aflow.org/p/8FHP>

[https://aflow.org/p/A2B11\\_cP39\\_200\\_f\\_begik-001](https://aflow.org/p/A2B11_cP39_200_f_begik-001)



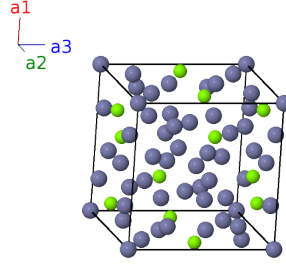
<b>Prototype</b>	Mg <sub>2</sub> Zn <sub>11</sub>
<b>AFLOW prototype label</b>	A2B11_cP39_200_f_begik-001
<b>Strukturbericht designation</b>	$D8_c$
<b>ICSD</b>	104898
<b>Pearson symbol</b>	cP39
<b>Space group number</b>	200
<b>Space group symbol</b>	$Pm\bar{3}$
<b>AFLOW prototype command</b>	aflow --proto=A2B11_cP39_200_f_begik-001 --params= $a, x_2, x_3, x_4, x_5, y_6, z_6$

## Other compounds with this structure

Na<sub>2</sub>Cd<sub>11</sub>, Mg<sub>2</sub>Cu<sub>6</sub>Al<sub>5</sub>, Mg<sub>2</sub>Cu<sub>6</sub>Ga<sub>5</sub>, Na<sub>2</sub>Au<sub>6</sub>In<sub>5</sub>, Sc<sub>2</sub>Co<sub>7</sub>Ga<sub>4</sub>, K<sub>6</sub>Na<sub>14</sub>CdTl<sub>18</sub>, K<sub>6</sub>Na<sub>14</sub>HgTl<sub>18</sub>, K<sub>6</sub>Na<sub>14</sub>MgTl<sub>18</sub>, K<sub>6</sub>Na<sub>14</sub>ZnTl<sub>18</sub>

## Simple Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(1b)	Zn I
$\mathbf{B}_2$	$= x_2 \mathbf{a}_1$	$=$	$ax_2 \hat{\mathbf{x}}$	(6e)	Zn II
$\mathbf{B}_3$	$= -x_2 \mathbf{a}_1$	$=$	$-ax_2 \hat{\mathbf{x}}$	(6e)	Zn II
$\mathbf{B}_4$	$= x_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{y}}$	(6e)	Zn II
$\mathbf{B}_5$	$= -x_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{y}}$	(6e)	Zn II
$\mathbf{B}_6$	$= x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{z}}$	(6e)	Zn II
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{z}}$	(6e)	Zn II
$\mathbf{B}_8$	$= x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f)	Mg I
$\mathbf{B}_9$	$= -x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6f)	Mg I
$\mathbf{B}_{10}$	$= \frac{1}{2} \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}}$	(6f)	Mg I
$\mathbf{B}_{11}$	$= \frac{1}{2} \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}}$	(6f)	Mg I
$\mathbf{B}_{12}$	$= \frac{1}{2} \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(6f)	Mg I
$\mathbf{B}_{13}$	$= \frac{1}{2} \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(6f)	Mg I
$\mathbf{B}_{14}$	$= x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6g)	Zn III
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6g)	Zn III
$\mathbf{B}_{16}$	$= x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6g)	Zn III
$\mathbf{B}_{17}$	$= -x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6g)	Zn III
$\mathbf{B}_{18}$	$= \frac{1}{2} \mathbf{a}_1 + x_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + ax_4 \hat{\mathbf{z}}$	(6g)	Zn III
$\mathbf{B}_{19}$	$= \frac{1}{2} \mathbf{a}_1 - x_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - ax_4 \hat{\mathbf{z}}$	(6g)	Zn III
$\mathbf{B}_{20}$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(8i)	Zn IV
$\mathbf{B}_{21}$	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(8i)	Zn IV
$\mathbf{B}_{22}$	$= -x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(8i)	Zn IV
$\mathbf{B}_{23}$	$= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(8i)	Zn IV
$\mathbf{B}_{24}$	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(8i)	Zn IV
$\mathbf{B}_{25}$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(8i)	Zn IV
$\mathbf{B}_{26}$	$= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(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

$$\begin{aligned}
\mathbf{B}_{31} &= \frac{1}{2} \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= & \frac{1}{2} a \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}} & (12k) & \text{Zn V} \\
\mathbf{B}_{32} &= z_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + y_6 \mathbf{a}_3 &= & az_6 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}} & (12k) & \text{Zn V} \\
\mathbf{B}_{33} &= z_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - y_6 \mathbf{a}_3 &= & az_6 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}} & (12k) & \text{Zn V} \\
\mathbf{B}_{34} &= -z_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + y_6 \mathbf{a}_3 &= & -az_6 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}} & (12k) & \text{Zn V} \\
\mathbf{B}_{35} &= -z_6 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - y_6 \mathbf{a}_3 &= & -az_6 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}} & (12k) & \text{Zn V} \\
\mathbf{B}_{36} &= y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & ay_6 \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (12k) & \text{Zn V} \\
\mathbf{B}_{37} &= -y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & -ay_6 \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (12k) & \text{Zn V} \\
\mathbf{B}_{38} &= y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & ay_6 \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (12k) & \text{Zn V} \\
\mathbf{B}_{39} &= -y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= & -ay_6 \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (12k) & \text{Zn V}
\end{aligned}$$

## References

- [1] S. Samson, *Die Kristallstruktur von Mg<sub>2</sub>Zn<sub>11</sub>*, Acta Chem. Scand. **3**, 835–843 (1949), doi:10.3891/acta.chem.scand.03-0835.