

D_{2_2} (MgZn₅?) Structure (*Problematic*): AB5_mC48_12_2i_ac5i2j-001

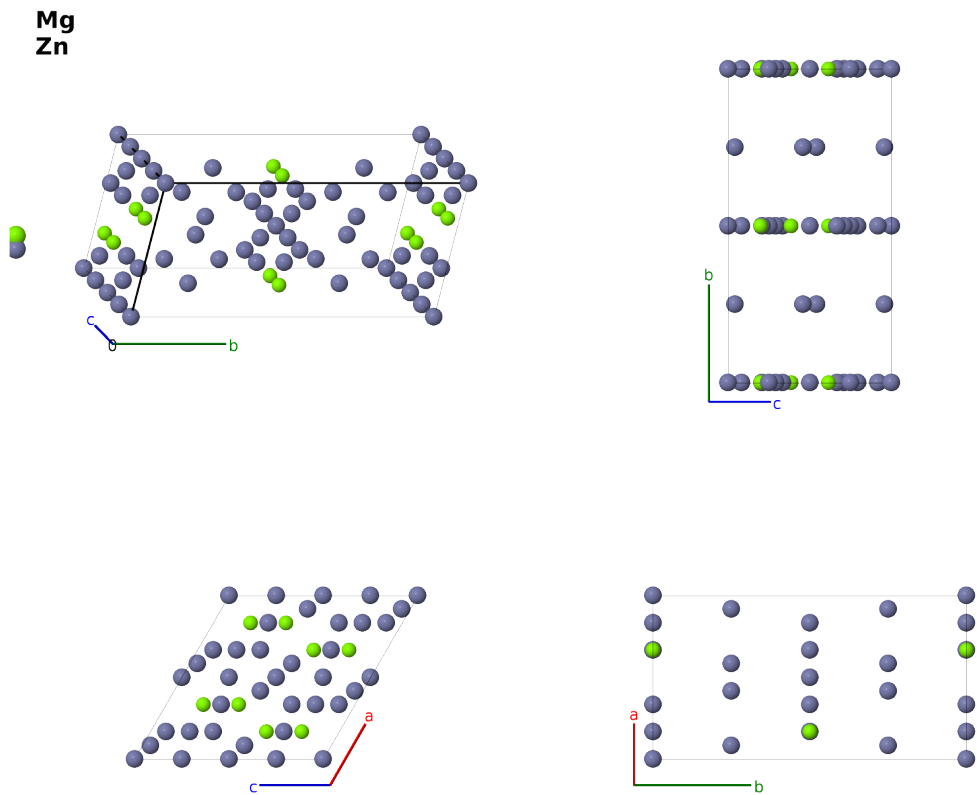
This structure previously used the label(s) AB5_mC48_12_2i_ac5i2j. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/5R9K>

https://aflow.org/prototype-encyclopedia/AB5_mC48_12_2i_ac5i2j-001



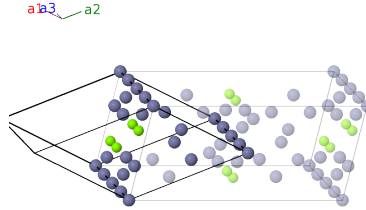
Prototype	MgZn ₅
AFLOW prototype label	AB5_mC48_12_2i_ac5i2j-001
<i>Strukturbericht</i> designation	D_{2_2}
ICSD	151403
CCDC	1668234
Pearson symbol	mC48
Space group number	12

Space group symbol	$C2/m$
AFLOW prototype command	<pre> aflow --proto=AB5_mC48_12_2i_ac5i2j-001 --params=a,b/a,c/a,β,x_3,z_3,x_4,z_4,x_5,z_5,x_6,z_6,x_7,z_7,x_8,z_8,x_9,z_9,x_{10},z_{10},x_{11},y_{11},z_{11} </pre>

- This structure has problems similar to the $B30$ MgZn structure, and for the same reasons. (Hermann, 1937) assigned this the *Strukturbericht* designation $D2_2$, based on the paper of (Tarschish, 1933), who derived it from the hexagonal Laves structure MgZn_2 ($C14$), eventually resulting in a 48 atom cell with composition MgZn_5 . As with MgZn , he assumed that the space group remained $P6_3/mmc$ #194.
- (McKeehan, 1935) again pointed out that this is impossible. (Hermann, 1937) referenced both papers, giving the space group as $P6_3/mmc$ but listing the atomic coordinates enumerated by McKeehan.
- The McKeehan structure has space group $C2/m$ #12, with 48 atoms in the conventional cell, and 24 atoms in the primitive cell. As with $B30$, this agrees with the structure (Parthé, 1993) designated as $D2_2$.
- It is not clear that any MgZn_5 compound actually exists. It does not appear in the assessed Mg-Zn binary phase diagram (Massalski, 1990). It *may* actually be the $\text{Mg}_2\text{Zn}_{11}$ $D8_c$ structure, but we have found no literature supporting this claim.
- The ICSD entry is from (Tarschish, 1933). It gives the atomic positions in space group $P1$ #1, but AFLOW finds that the structure is in space group $C2/m$ #12, as found from our analysis of (McKeehan, 1935). Unsurprisingly, this structure does not agree with our interpretation of the data.

Base-centered Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(2a) Zn I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(2c) Zn II
$\mathbf{B}_3$	$=$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Mg I
$\mathbf{B}_4$	$=$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Mg I
$\mathbf{B}_5$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) Mg II
$\mathbf{B}_6$	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) Mg II
$\mathbf{B}_7$	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4i) Zn III
$\mathbf{B}_8$	$=$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4i) Zn III
$\mathbf{B}_9$	$=$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4i) Zn IV
$\mathbf{B}_{10}$	$=$	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4i) Zn IV
$\mathbf{B}_{11}$	$=$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4i) Zn V

$\mathbf{B}_{12}$	$= -x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4i)	Zn V
$\mathbf{B}_{13}$	$= x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4i)	Zn VI
$\mathbf{B}_{14}$	$= -x_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(4i)	Zn VI
$\mathbf{B}_{15}$	$= x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(4i)	Zn VII
$\mathbf{B}_{16}$	$= -x_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(4i)	Zn VII
$\mathbf{B}_{17}$	$= \begin{matrix} (x_{10} - y_{10}) \mathbf{a}_1 + \\ (x_{10} + y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 \end{matrix}$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(8j)	Zn VIII
$\mathbf{B}_{18}$	$= \begin{matrix} -(x_{10} + y_{10}) \mathbf{a}_1 - \\ (x_{10} - y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3 \end{matrix}$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - \\ cz_{10} \sin \beta \hat{\mathbf{z}}$	(8j)	Zn VIII
$\mathbf{B}_{19}$	$= \begin{matrix} -(x_{10} - y_{10}) \mathbf{a}_1 - \\ (x_{10} + y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3 \end{matrix}$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - \\ cz_{10} \sin \beta \hat{\mathbf{z}}$	(8j)	Zn VIII
$\mathbf{B}_{20}$	$= \begin{matrix} (x_{10} + y_{10}) \mathbf{a}_1 + \\ (x_{10} - y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 \end{matrix}$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(8j)	Zn VIII
$\mathbf{B}_{21}$	$= \begin{matrix} (x_{11} - y_{11}) \mathbf{a}_1 + \\ (x_{11} + y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3 \end{matrix}$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(8j)	Zn IX
$\mathbf{B}_{22}$	$= \begin{matrix} -(x_{11} + y_{11}) \mathbf{a}_1 - \\ (x_{11} - y_{11}) \mathbf{a}_2 - z_{11} \mathbf{a}_3 \end{matrix}$	$=$	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} - \\ cz_{11} \sin \beta \hat{\mathbf{z}}$	(8j)	Zn IX
$\mathbf{B}_{23}$	$= \begin{matrix} -(x_{11} - y_{11}) \mathbf{a}_1 - \\ (x_{11} + y_{11}) \mathbf{a}_2 - z_{11} \mathbf{a}_3 \end{matrix}$	$=$	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} - \\ cz_{11} \sin \beta \hat{\mathbf{z}}$	(8j)	Zn IX
$\mathbf{B}_{24}$	$= \begin{matrix} (x_{11} + y_{11}) \mathbf{a}_1 + \\ (x_{11} - y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3 \end{matrix}$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(8j)	Zn IX

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