$D2_2$ ($MgZn_5$?) Structure (*Problematic*): AB5_mC48_12_2i_ac5i2j-001

This structure originally had the label `AB5_mC48_12_2i_ac5i2j`. Calls to that address will be redirected here.

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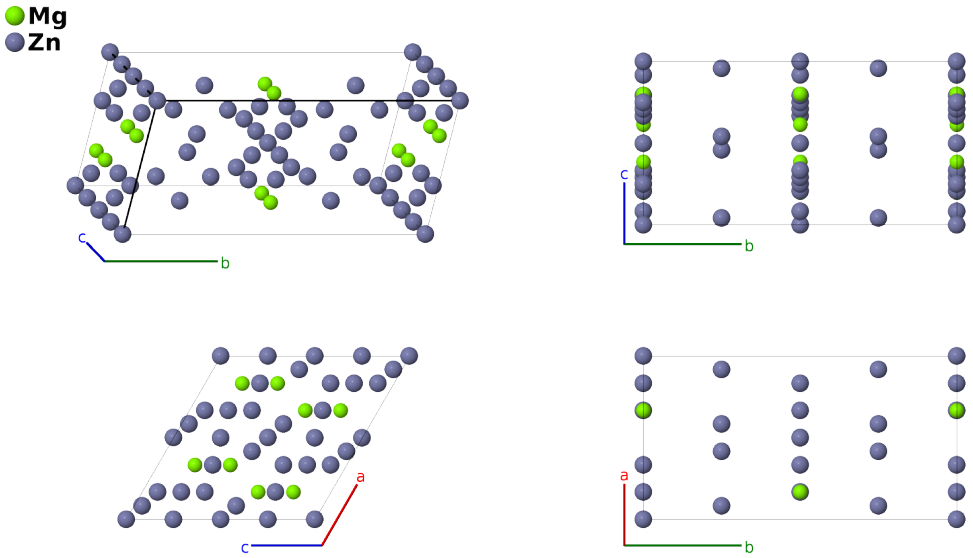
https://aflow.org/p/5R9K

https://aflow.org/p/AB5_mC48_12_2i_ac5i2j-001



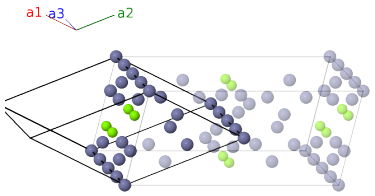
Prototype	$MgZn_5$
AFLOW prototype label	AB5_mC48_12_2i_ac5i2j-001
***Strukturbericht* designation**	$D2_2$
ICSD	151403
Pearson symbol	mC48
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=AB5_mC48_12_2i_ac5i2j-001 --params=`$a, b/a, c/a, \beta, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}$

- 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 Mg_2Zn_{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

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}\\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}\\ \mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}\end{aligned}$$



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
$\mathbf{B_{17}}$	=	$(x_{10} - y_{10})\,\mathbf{a}_1 + (x_{10} + y_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Zn VIII
$\mathbf{B_{18}}$	=	$-(x_{10} + y_{10})\,\mathbf{a}_1 - (x_{10} - y_{10})\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Zn VIII
$\mathbf{B_{19}}$	=	$-(x_{10} - y_{10})\,\mathbf{a}_1 - (x_{10} + y_{10})\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Zn VIII
$\mathbf{B_{20}}$	=	$(x_{10} + y_{10})\,\mathbf{a}_1 + (x_{10} - y_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Zn VIII
$\mathbf{B_{21}}$	=	$(x_{11} - y_{11})\,\mathbf{a}_1 + (x_{11} + y_{11})\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Zn IX

$\mathbf{B_{22}}$	=	$-(x_{11}+y_{11})\,\mathbf{a}_1 -$ $(x_{11}-y_{11})\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-(ax_{11}+cz_{11}\cos\beta)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} -$ $cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Zn IX
$\mathbf{B_{23}}$	=	$-(x_{11}-y_{11})\,\mathbf{a}_1 -$ $(x_{11}+y_{11})\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-(ax_{11}+cz_{11}\cos\beta)\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} -$ $cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Zn IX
$\mathbf{B_{24}}$	=	$(x_{11}+y_{11})\,\mathbf{a}_1 +$ $(x_{11}-y_{11})\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11}+cz_{11}\cos\beta)\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Zn IX

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