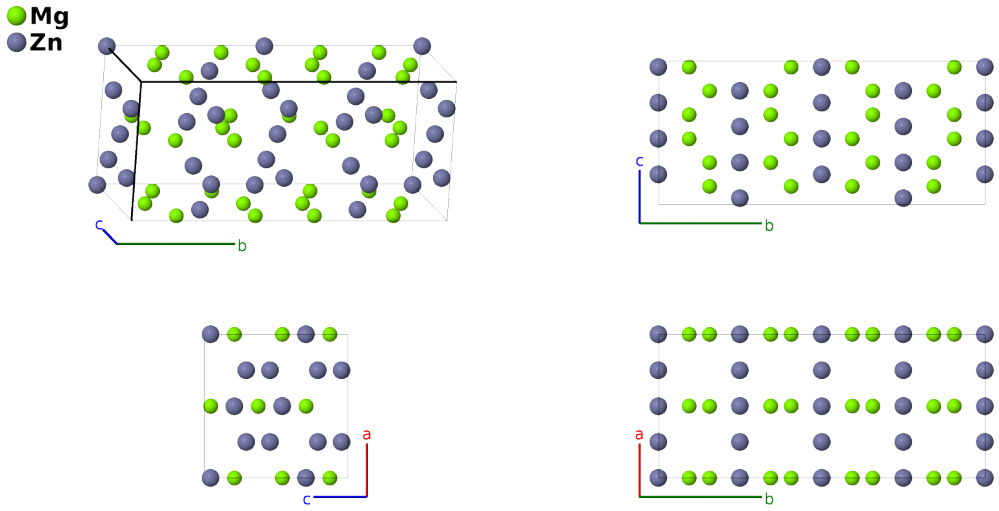
$B30$ (MgZn?) Structure (*Problematic*): AB_oI48_44_6c_abc2de-001

This structure originally had the label `AB_oI48_44_6d_ab2cde`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

https://aflow.org/p/WDVJ

https://aflow.org/p/AB_oI48_44_6c_abc2de-001



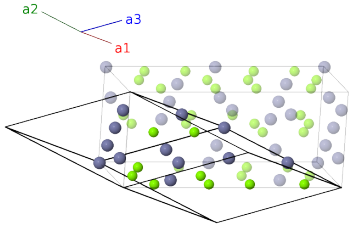
Prototype	MgZn
AFLOW prototype label	AB_oI48_44_6c_abc2de-001
***Strukturbericht* designation**	$B30$
ICSD	151402
Pearson symbol	oI48
Space group number	44
Space group symbol	$Imm2$
AFLOW prototype command	`aflow --proto=AB_oI48_44_6c_abc2de-001 --params=`$a, b/a, c/a, z_1, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, y_{10}, z_{10}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}$

- It is rather a mystery why (Hermann, 1937) gave this the *Strukturbericht* designation $B30$, as the structure presented in the literature contradicts itself. (Tarschish, 1933) derived this structure from the hexagonal Laves structure $MgZn_2$ (C14) by doubling the unit cell in all directions to obtain a 96 atom unit cell, replacing 16 of the zinc atoms in this structure by magnesium, and shifting the z-coordinates of these atoms by $\pm c/16$. He then states that the space group remains $P6_3/mmc$ #194.
- (McKeehan, 1935) pointed out that this is impossible, as the converted Mg atoms only have a two-fold rotation axis about the z-axis. He assigned the structure to space group $Pmm2$ #25.

- (Hermann, 1937) referenced both papers, giving the space group as $P6_3/mmc$ but listing the atomic coordinates enumerated by McKeehan.
- In fact, the McKeehan structure has space group $Imm2$ #44, with 48 atoms in the conventional cell, half of the original, and 24 atoms in the primitive cell. This was noted, without reference, by (Parthé, 1993), which is the only comprehensive list of *Strukturbericht* symbols to include the $B30$ structure. We have reproduced this $Imm2$ structure from McKeehan's data.
- The true structure of MgZn is unclear. It is seen in the Mg-Zn binary phase diagram (Massalski, 1990) over a small range of compositions, but a complete crystallographic study has never been published. It is possible that the actual structure is off-stoichiometry. There is some evidence of an $Mg_{12}Zn_{13}$ structure (Mezbahul-Islam, 2014), and $Mg_{21}Zn_{25}$ has been determined (Cerný, 2002) to have the $Zr_{21}Re_{25}$ structure.
- There are similar problems with the $D2_2$ $MgZn_5$ structure, which we discuss on that page.
- 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 $Imm2$ #44, as found from our analysis of (McKeehan, 1935). Unsurprisingly, this structure does not agree with our interpretation of the data.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Zn I
$\mathbf{B_2}$	=	$\left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2b)	Zn II
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(4c)	Mg I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(4c)	Mg I
$\mathbf{B_5}$	=	$z_4\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(4c)	Mg II
$\mathbf{B_6}$	=	$z_4\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(4c)	Mg II
$\mathbf{B_7}$	=	$z_5\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(4c)	Mg III
$\mathbf{B_8}$	=	$z_5\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(4c)	Mg III
$\mathbf{B_9}$	=	$z_6\,\mathbf{a}_1 + (x_6 + z_6)\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(4c)	Mg IV
$\mathbf{B_{10}}$	=	$z_6\,\mathbf{a}_1 - (x_6 - z_6)\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(4c)	Mg IV
$\mathbf{B_{11}}$	=	$z_7\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + cz_7\,\hat{\mathbf{z}}$	(4c)	Mg V
$\mathbf{B_{12}}$	=	$z_7\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + cz_7\,\hat{\mathbf{z}}$	(4c)	Mg V
$\mathbf{B_{13}}$	=	$z_8\,\mathbf{a}_1 + (x_8 + z_8)\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + cz_8\,\hat{\mathbf{z}}$	(4c)	Mg VI
$\mathbf{B_{14}}$	=	$z_8\,\mathbf{a}_1 - (x_8 - z_8)\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + cz_8\,\hat{\mathbf{z}}$	(4c)	Mg VI
$\mathbf{B_{15}}$	=	$z_9\,\mathbf{a}_1 + (x_9 + z_9)\,\mathbf{a}_2 + x_9\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} + cz_9\,\hat{\mathbf{z}}$	(4c)	Zn III
$\mathbf{B_{16}}$	=	$z_9\,\mathbf{a}_1 - (x_9 - z_9)\,\mathbf{a}_2 - x_9\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} + cz_9\,\hat{\mathbf{z}}$	(4c)	Zn III
$\mathbf{B_{17}}$	=	$(y_{10} + z_{10})\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 + y_{10}\,\mathbf{a}_3$	=	$by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(4d)	Zn IV
$\mathbf{B_{18}}$	=	$-(y_{10} - z_{10})\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 - y_{10}\,\mathbf{a}_3$	=	$-by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(4d)	Zn IV
$\mathbf{B_{19}}$	=	$(y_{11} + z_{11})\,\mathbf{a}_1 + z_{11}\,\mathbf{a}_2 + y_{11}\,\mathbf{a}_3$	=	$by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(4d)	Zn V

$\mathbf{B_{20}}$	=	$-(y_{11}-z_{11})\,\mathbf{a}_1+z_{11}\,\mathbf{a}_2-y_{11}\,\mathbf{a}_3$	=	$-by_{11}\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}}$	(4d)	Zn V
$\mathbf{B_{21}}$	=	$(y_{12}+z_{12})\,\mathbf{a}_1+(x_{12}+z_{12})\,\mathbf{a}_2+(x_{12}+y_{12})\,\mathbf{a}_3$	=	$ax_{12}\,\hat{\mathbf{x}}+by_{12}\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}}$	(8e)	Zn VI
$\mathbf{B_{22}}$	=	$-(y_{12}-z_{12})\,\mathbf{a}_1-(x_{12}-z_{12})\,\mathbf{a}_2-(x_{12}+y_{12})\,\mathbf{a}_3$	=	$-ax_{12}\,\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}}$	(8e)	Zn VI
$\mathbf{B_{23}}$	=	$-(y_{12}-z_{12})\,\mathbf{a}_1+(x_{12}+z_{12})\,\mathbf{a}_2+(x_{12}-y_{12})\,\mathbf{a}_3$	=	$ax_{12}\,\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}}$	(8e)	Zn VI
$\mathbf{B_{24}}$	=	$(y_{12}+z_{12})\,\mathbf{a}_1-(x_{12}-z_{12})\,\mathbf{a}_2-(x_{12}-y_{12})\,\mathbf{a}_3$	=	$-ax_{12}\,\hat{\mathbf{x}}+by_{12}\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}}$	(8e)	Zn VI

References

[1] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

[2] L. Tarschisch, *Röntgenographische Untersuchung der Verbindungen MgZn und $MgZn_5$*, Z. Kristallogr. **86**, 423–438 (1933), doi:10.1524/zkri.1933.86.1.423.

[3] L. W. McKeehan, *Note on MgZn and $MgZn_5$*, Z. Kristallogr. **91**, 501–503 (1935), doi:10.1524/zkri.1935.91.1.501.

[4] E. Parthé, L. Gelato, B. Chabot, M. Penso, K. Cenzula, and R. Gladyshevskii, *Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types*, *Gmelin Handbook of Inorganic and Organometallic Chemistry*, vol. 2 (Springer-Verlag, Berlin, Heidelberg, 1993), 8 edn., doi:10.1007/978-3-662-02909-1_3.

[5] T. B. Massalski, H. Okamoto, P. R. Subramanian, and L. Kacprzak, eds., *Binary Alloy Phase Diagrams*, vol. 3 (ASM International, Materials Park, Ohio, USA, 1990), 2^{nd} edn. Hf-Re to Zn-Zr.

[6] M. Mezbahul-Islam, A. O. Mostafa, and M. Medraj, *Essential Magnesium Alloys Binary Phase Diagrams and Their Thermochemical Data*, J. Mater. **2014**, 704283 (2014), doi:10.1155/2014/704283.

[7] R. Cerný and G. Renaudin, *The intermetallic compound $Mg_{21}Zn_{25}$*, Acta Crystallogr. Sect. C **58**, i154–i155 (2002), doi:10.1107/S0108270102018103.