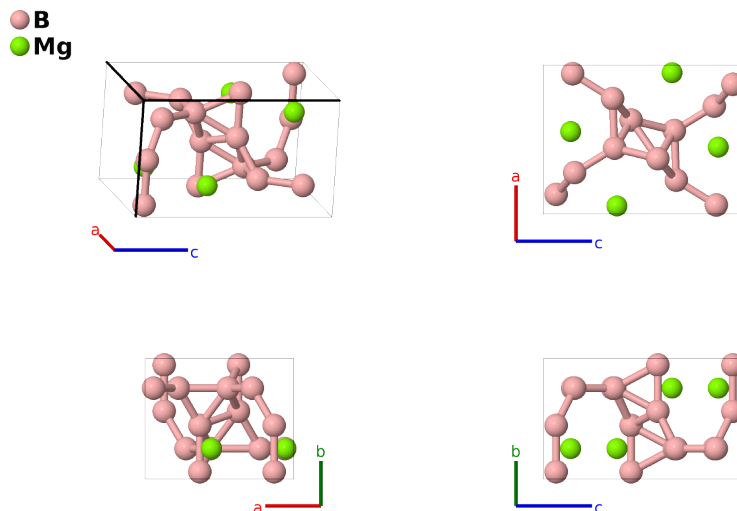# MgB$_4$ Structure:
A4B_oP20_62_2cd_c-001

This structure originally had the label `A4B_oP20_62_2cd_c`. Calls to that address will be redirected here.

https://aflow.org/p/8U8B

https://aflow.org/p/A4B_oP20_62_2cd_c-001

Prototype	B$_4$Mg
AFLOW prototype label	A4B_oP20_62_2cd_c-001
ICSD	23460
Pearson symbol	oP20
Space group number	62
Space group symbol	$Pnma$
AFLOW prototype command	aflow --proto=A4B_oP20_62_2cd_c-001 --params=$a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, z_3, x_4, y_4, z_4$

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
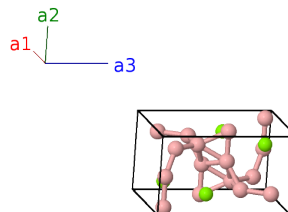
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	$=$	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B_2}$	$=$	$-\left(x_1 - \frac{1}{2}\right)\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B_3}$	$=$	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 - z_1\,\mathbf{a}_3$	$=$	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B_4}$	$=$	$\left(x_1 + \frac{1}{2}\right)\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B_5}$	$=$	$x_2\,\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + z_2\,\mathbf{a}_3$	$=$	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	B II
$\mathbf{B_6}$	$=$	$-\left(x_2 - \frac{1}{2}\right)\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	B II
$\mathbf{B_7}$	$=$	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 - z_2\,\mathbf{a}_3$	$=$	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4c)	B II
$\mathbf{B_8}$	$=$	$\left(x_2 + \frac{1}{2}\right)\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	B II
$\mathbf{B_9}$	$=$	$x_3\,\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + z_3\,\mathbf{a}_3$	$=$	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	Mg I
$\mathbf{B_{10}}$	$=$	$-\left(x_3 - \frac{1}{2}\right)\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Mg I
$\mathbf{B_{11}}$	$=$	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 - z_3\,\mathbf{a}_3$	$=$	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4c)	Mg I
$\mathbf{B_{12}}$	$=$	$\left(x_3 + \frac{1}{2}\right)\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right)\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Mg I
$\mathbf{B_{13}}$	$=$	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8d)	B III
$\mathbf{B_{14}}$	$=$	$-\left(x_4 - \frac{1}{2}\right)\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right)\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	B III
$\mathbf{B_{15}}$	$=$	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\mathbf{a}_2 - z_4\,\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8d)	B III
$\mathbf{B_{16}}$	$=$	$\left(x_4 + \frac{1}{2}\right)\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	B III
$\mathbf{B_{17}}$	$=$	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8d)	B III
$\mathbf{B_{18}}$	$=$	$\left(x_4 + \frac{1}{2}\right)\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	B III
$\mathbf{B_{19}}$	$=$	$x_4\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\mathbf{a}_2 + z_4\,\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8d)	B III
$\mathbf{B_{20}}$	$=$	$-\left(x_4 - \frac{1}{2}\right)\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8d)	B III

References

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[2] A. Guette, R. Naslain, and J. Galy, *Structure cristalline de tetraborure de magnesium*, C. R. Acad. Sci. Series C **275**, 41–44 (1972).

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