$MgZn_2$ Hexagonal Laves ($C14$) Structure: AB2_hP12_194_f_ah-001

This structure originally had the label `AB2_hP12_194_f_ah`. Calls to that address will be redirected here.

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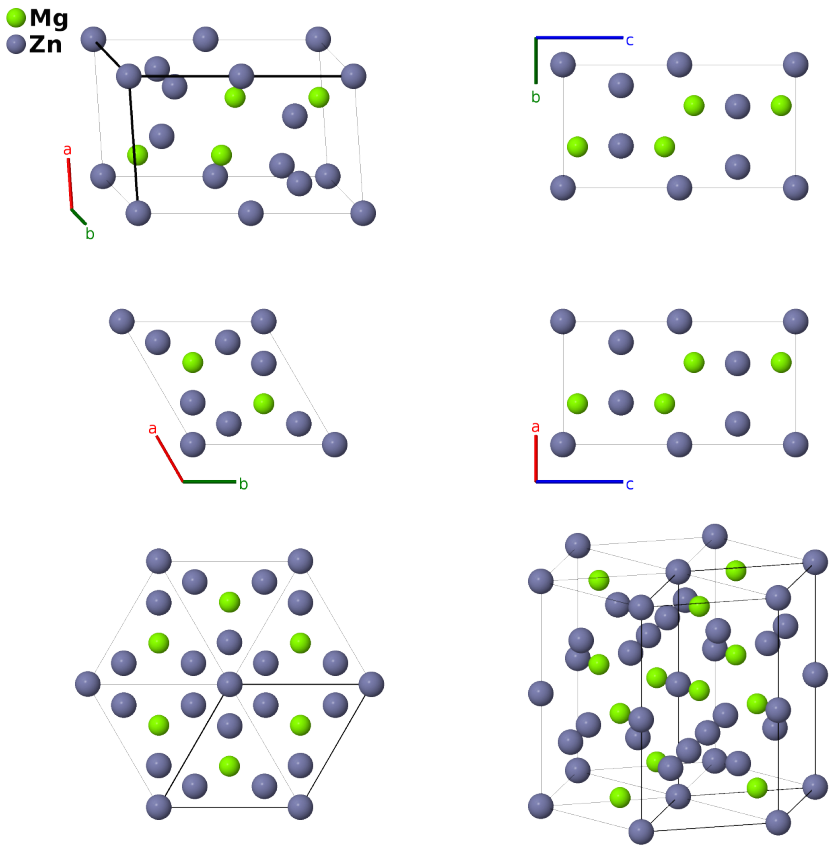
https://aflow.org/p/LL0C

https://aflow.org/p/AB2_hP12_194_f_ah-001



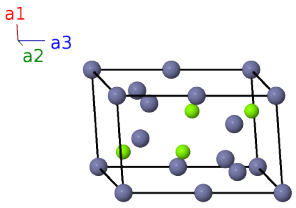
Prototype	$MgZn_2$
AFLOW prototype label	AB2_hP12_194_f_ah-001
***Strukturbericht* designation**	$C14$
Mineral name	Hexagonal Laves
ICSD	46006
Pearson symbol	hP12
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=AB2_hP12_194_f_ah-001 --params=`$a, c/a, z_2, x_3$

Other compounds with this structure

$BaMg_2$, $CaCd_2$, $CaLi_2$, $CaMg_2$, $CdCu_2$, $CrBe_2$, $DyOs_2$, $DyRu_2$, $DyTc_2$, $ErMg_2$, $ErMn_2$, $ErOs_2$, $ErRu_2$, $ErTc_2$, $FeBe_2$, $GdOs_2$, $GdRu_2$, $GdTc_2$, $HfCr_2$, $HfFe_2$ (HT), $HfMn_2$ (HT), $HfRe_2$, $HoMg_2$, $HoOs_2$, $HoRe_2$, $HoRu_2$, $HoTc_2$, KNa_2, KPb_2, $LuMn_2$, $LuOs_2$, $LuRe_2$, $LuRh_2$, $LuRu_2$, $LuTe_2$, $MgZn_2$, $MnBe_2$, $MoBe_2$, $MoFe_2$, $NbCr_2$ (HT), $NbFe_2$, $NbMn_2$, $NdMn_2$, $NdOs_2$, $PrMn_2$, $PrOs_2$, $PuOs_2$, $ReBe_2$, $RuBe_2$, $ScMn_2$, $ScOs_2$, $ScRe_2$, $ScRu_2$, $ScTc_2$, $SmOs_2$, $SrMg_2$, α-$TaCo_2$ (LT), $TaCr_2$ (HT), $TaFe_2$, $TaMn_2$, $TbOs_2$, $TbRe_2$, $TbRu_2$, $TbTc_2$, $ThMn_2$, $ThRe_2$, $TiCr_2$ (HT), $TiFe_2$, $TiMn_2$, $TiZn_2$, $TmMn_2$, $TmRu_2$, $TmTc_2$, UNi_2, URe_2 (HT), URe_2, VBe_2, WBe_2, WFe_2, YOs_2, YRe_2, YRu_2, YTc_2, $ZrCr_2$, $ZrMn_2$, $ZrOs_2$, $ZrRe_2$, $ZrRu_2$ (HT), $ZrTc_2$, Co_3Mn_2Ge, Co_3Mo_2Si, Cr_3Ta_2Cu, Fe_3Zr_2Ga, Nb_3Co_2Si, Ni_3Nb_2Si, Ni_3Ta_2Si, Ni_3Ti_2Si

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}\\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}\\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Zn I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Zn I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4f)	Mg I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Mg I
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4f)	Mg I
$\mathbf{B_6}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Mg I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Zn II
$\mathbf{B_8}$	=	$-2x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Zn II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Zn II
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - 2x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Zn II
$\mathbf{B_{11}}$	=	$2x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Zn II
$\mathbf{B_{12}}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\sqrt{3}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Zn II

References

[1] T. Ohba, Y. Kitano, and Y. Komura, *The charge-density study of the Laves phases, $MgZn_2$ and $MgCu_2$*, Acta Crystallogr. Sect. C **40**, 1–5 (1984), doi:10.1107/S0108270184002791.