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

This structure previously used the label(s) `AB2_hP12_194_f_ah`. Calls to these addresses will be redirected here.

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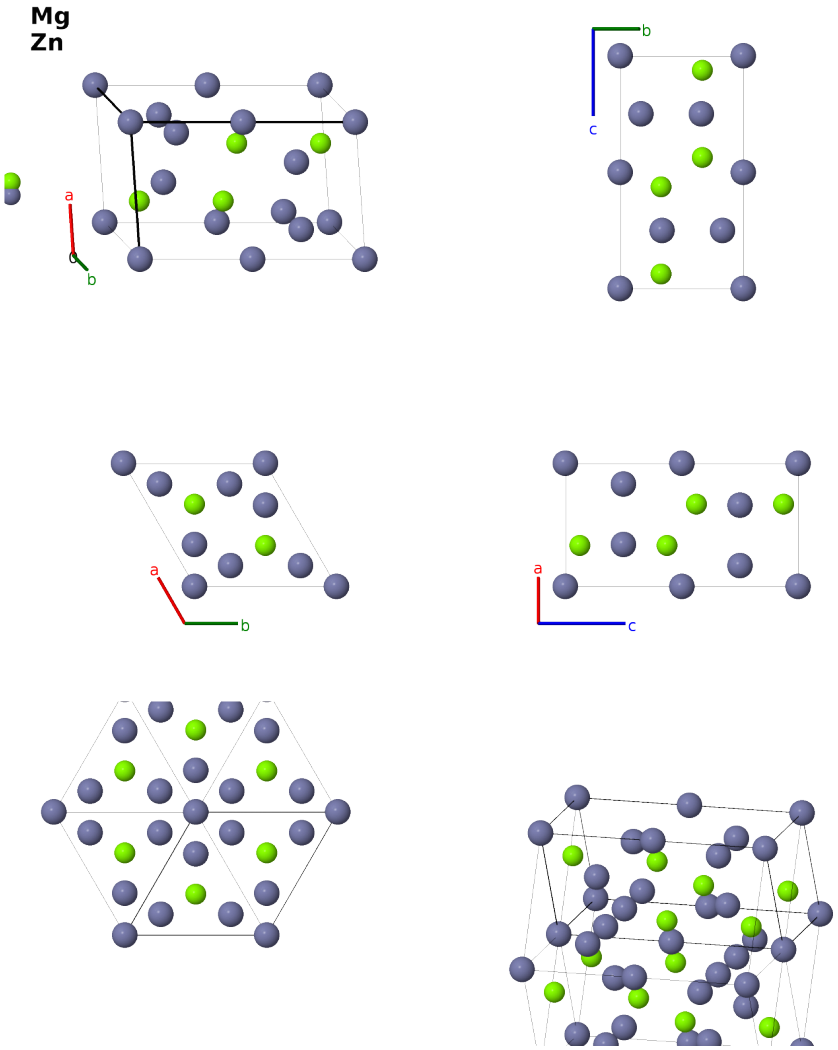
https://aflow.org/prototype-encyclopedia/LL0C

https://aflow.org/prototype-encyclopedia/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 |
| **CCDC** | 1614392 |
| **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=`$a, c/a, z_2, x_3$ |

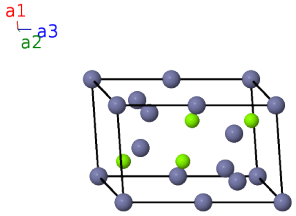
**Other compounds with this structure**

$BaMg_2$, $CaCd_2$, $CaLi_2$, $CaMg_2$, $CdCu_2$, $CrBe_2$, $DyOs_2$, $DyRu_2$, $DyTc_2$, $ErMg_2$, $ErMn_2$, $ErOs_2$, $ErRu_2$, $ErTc_2$, $FeBe_2$, $GdOs_2$, $GdRu_2$, $GdTc_2$, $HfCr_2$, $HfFe_2$ (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), $NbFe_2$, $NbMn_2$, $NdMn_2$, $NdOs_2$, $PrMn_2$, $PrOs_2$, $PuOs_2$, $ReBe_2$, $RuBe_2$, $ScMn_2$, $ScOs_2$, $ScRe_2$, $ScRu_2$, $ScTc_2$, $SmOs_2$, $SrMg_2$, $\alpha$-$TaCo_2$ (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), $ZrTc_2$

- $U_2Cr_3Si$ is a ternary form of this structure.

**Hexagonal primitive vectors**

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$




**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.

## First cited in

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