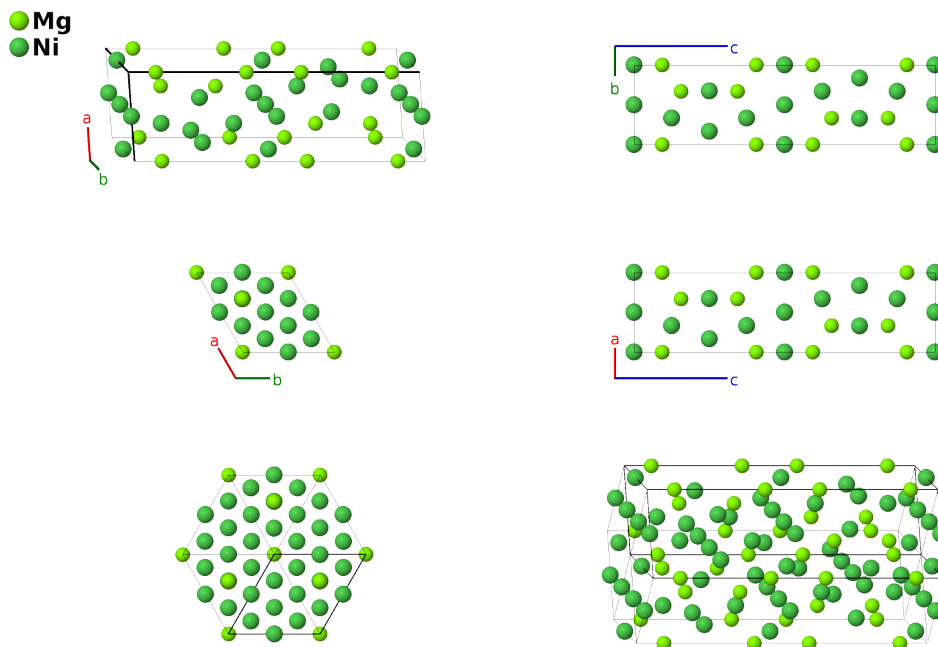# MgNi$_2$ Hexagonal Laves ($C36$) Structure: AB2_hP24_194_ef_fgh-001

This structure originally had the label `AB2_hP24_194_ef_fgh`. Calls to that address will be redirected here.

https://aflow.org/p/HV5V

https://aflow.org/p/AB2_hP24_194_ef_fgh-001

Prototype	MgNi$_2$
AFLOW prototype label	AB2_hP24_194_ef_fgh-001
Strukturbericht designation	$C36$
ICSD	104838
Pearson symbol	hP24
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=AB2_hP24_194_ef_fgh-001` `           --params=`$a, c/a, z_1, z_2, z_3, x_5$

Other compounds with this structure

CdCu$_2$, HfCr$_2$, HfFe$_2$, HfMo$_2$ (HT), NbCo$_2$, NbZn$_2$, ScFe$_2$, ThMg$_2$ (LT), β-TiCo$_2$, UPt$_2$

- An AFLOW user, Mehdi Noori, identified an inconsistency with this entry and the original reference (Mehl, 2017): the z-value for Mg (I) 4e should have been 0.09400, not 0.04598. This entry has been corrected.

Hexagonal primitive vectors

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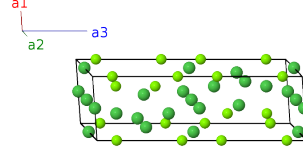
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$z_1\,\mathbf{a_3}$	$=$	$cz_1\,\hat{\mathbf{z}}$	(4e)	Mg I
$\mathbf{B_2}$	$=$	$\left(z_1 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$c\left(z_1 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4e)	Mg I
$\mathbf{B_3}$	$=$	$-z_1\,\mathbf{a_3}$	$=$	$-cz_1\,\hat{\mathbf{z}}$	(4e)	Mg I
$\mathbf{B_4}$	$=$	$-\left(z_1 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-c\left(z_1 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4e)	Mg I
$\mathbf{B_5}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4f)	Mg II
$\mathbf{B_6}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \left(z_2 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4f)	Mg II
$\mathbf{B_7}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} - z_2\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4f)	Mg II
$\mathbf{B_8}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} - \left(z_2 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_2 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4f)	Mg II
$\mathbf{B_9}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4f)	Ni I
$\mathbf{B_{10}}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \left(z_3 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4f)	Ni I
$\mathbf{B_{11}}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4f)	Ni I
$\mathbf{B_{12}}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} - \left(z_3 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4f)	Ni I
$\mathbf{B_{13}}$	$=$	$\tfrac{1}{2}\mathbf{a_1}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(6g)	Ni II
$\mathbf{B_{14}}$	$=$	$\tfrac{1}{2}\mathbf{a_2}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(6g)	Ni II
$\mathbf{B_{15}}$	$=$	$\tfrac{1}{2}\mathbf{a_1} + \tfrac{1}{2}\mathbf{a_2}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}}$	(6g)	Ni II
$\mathbf{B_{16}}$	$=$	$\tfrac{1}{2}\mathbf{a_1} + \tfrac{1}{2}\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Ni II
$\mathbf{B_{17}}$	$=$	$\tfrac{1}{2}\mathbf{a_2} + \tfrac{1}{2}\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Ni II
$\mathbf{B_{18}}$	$=$	$\tfrac{1}{2}\mathbf{a_1} + \tfrac{1}{2}\mathbf{a_2} + \tfrac{1}{2}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Ni II
$\mathbf{B_{19}}$	$=$	$x_5\,\mathbf{a_1} + 2x_5\,\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{3}{2}ax_5\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Ni III
$\mathbf{B_{20}}$	$=$	$-2x_5\,\mathbf{a_1} - x_5\,\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$-\tfrac{3}{2}ax_5\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Ni III
$\mathbf{B_{21}}$	$=$	$x_5\,\mathbf{a_1} - x_5\,\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$-\sqrt{3}ax_5\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Ni III
$\mathbf{B_{22}}$	$=$	$-x_5\,\mathbf{a_1} - 2x_5\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$-\tfrac{3}{2}ax_5\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Ni III
$\mathbf{B_{23}}$	$=$	$2x_5\,\mathbf{a_1} + x_5\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{3}{2}ax_5\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Ni III
$\mathbf{B_{24}}$	$=$	$-x_5\,\mathbf{a_1} + x_5\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\sqrt{3}ax_5\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Ni III

References

[1] Y. Komura and K. Tokunaga, *Structural studies of stacking variants in Mg-base Friauf-Laves phases*, Acta Crystallogr. Sect. B **36**, 1548–1554 (1980), doi:10.1107/S0567740880006565.

[2] M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1–S828 (2017), doi:10.1016/j.commatsci.2017.01.017.