# $Mg_2Ni$ ($C_a$) Structure: A2B_hP18_180_fj_ac-001

This structure previously used the label(s) `A2B_hP18_180_fi_bd`. Calls to these addresses will be redirected here.

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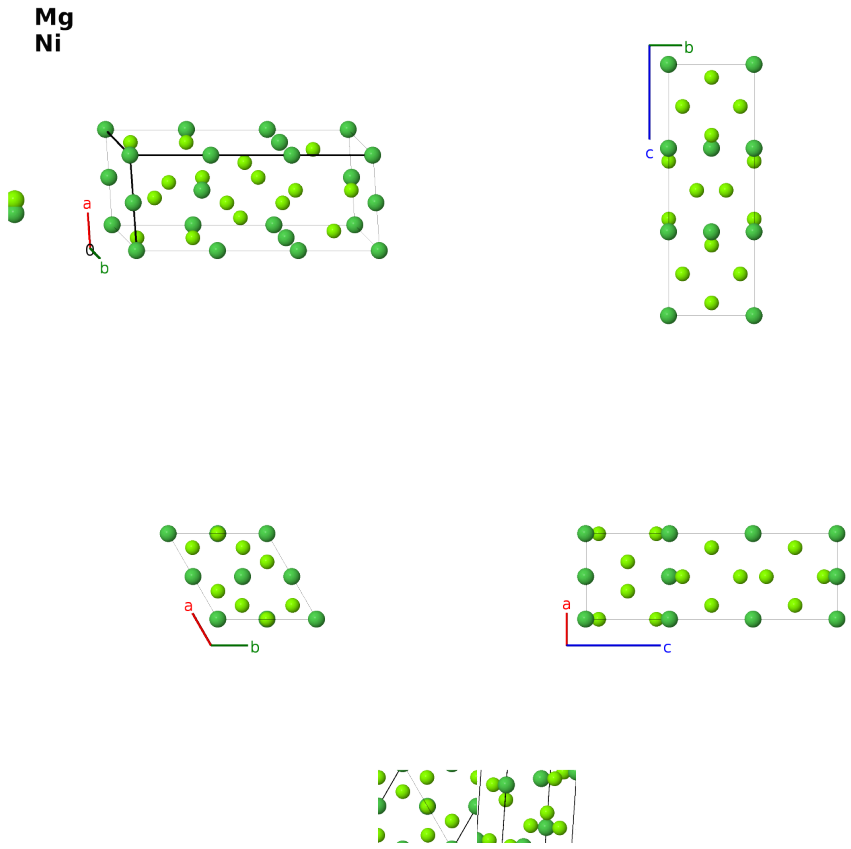
https://aflow.org/prototype-encyclopedia/TDY8

https://aflow.org/prototype-encyclopedia/A2B_hP18_180_fj_ac-001




| | |
|---|---|
| **Prototype** | $Mg_2Ni$ |
| **AFLOW prototype label** | A2B_hP18_180_fj_ac-001 |
| ***Strukturbericht* designation** | $C_a$ |
| **ICSD** | 104912 |
| **CCDC** | 1662813 |
| **Pearson symbol** | hP18 |
| **Space group number** | 180 |
| **Space group symbol** | $P6_222$ |

**AFLOW prototype command** `aflow --proto=A2B_hP18_180_fj_ac-001 --params=`$a, c/a, z_3, x_4$

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**Other compounds with this structure**

$CuMg_4Ni$, $MoSn_2$

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- This structure can also be found in the enantiomorphic space group $P6_422$ #181.
- Our original (Mehl, 2017) rendering of this structure swapped the magnesium $z_3$ and $x_4$ coordinates.

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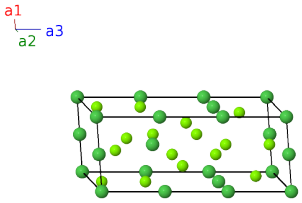
**Hexagonal primitive vectors**

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

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (3a) | Ni I |
| $\mathbf{B_2}$ | = | $\frac{2}{3}\,\mathbf{a}_3$ | = | $\frac{2}{3}c\,\hat{\mathbf{z}}$ | (3a) | Ni I |
| $\mathbf{B_3}$ | = | $\frac{1}{3}\,\mathbf{a}_3$ | = | $\frac{1}{3}c\,\hat{\mathbf{z}}$ | (3a) | Ni I |
| $\mathbf{B_4}$ | = | $\frac{1}{2}\,\mathbf{a}_1$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$ | (3c) | Ni II |
| $\mathbf{B_5}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + \frac{2}{3}\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{2}{3}c\,\hat{\mathbf{z}}$ | (3c) | Ni II |
| $\mathbf{B_6}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{3}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{3}c\,\hat{\mathbf{z}}$ | (3c) | Ni II |
| $\mathbf{B_7}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (6f) | Mg I |
| $\mathbf{B_8}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + \left(z_3 + \frac{2}{3}\right)\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_3 + 2)\,\hat{\mathbf{z}}$ | (6f) | Mg I |
| $\mathbf{B_9}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{3}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + c\left(z_3 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$ | (6f) | Mg I |
| $\mathbf{B_{10}}$ | = | $\frac{1}{2}\,\mathbf{a}_2 - \left(z_3 - \frac{2}{3}\right)\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} - \frac{1}{3}c\,(3z_3 - 2)\,\hat{\mathbf{z}}$ | (6f) | Mg I |
| $\mathbf{B_{11}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 - z_3\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (6f) | Mg I |
| $\mathbf{B_{12}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{3}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - c\left(z_3 - \frac{1}{3}\right)\,\hat{\mathbf{z}}$ | (6f) | Mg I |
| $\mathbf{B_{13}}$ | = | $x_4\,\mathbf{a}_1 + 2x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (6j) | Mg II |
| $\mathbf{B_{14}}$ | = | $-2x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{6}\,\mathbf{a}_3$ | = | $-\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$ | (6j) | Mg II |
| $\mathbf{B_{15}}$ | = | $x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{5}{6}\,\mathbf{a}_3$ | = | $-\sqrt{3}ax_4\,\hat{\mathbf{y}} + \frac{5}{6}c\,\hat{\mathbf{z}}$ | (6j) | Mg II |
| $\mathbf{B_{16}}$ | = | $-x_4\,\mathbf{a}_1 - 2x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (6j) | Mg II |
| $\mathbf{B_{17}}$ | = | $2x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{1}{6}\,\mathbf{a}_3$ | = | $\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$ | (6j) | Mg II |
| $\mathbf{B_{18}}$ | = | $-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{5}{6}\,\mathbf{a}_3$ | = | $\sqrt{3}ax_4\,\hat{\mathbf{y}} + \frac{5}{6}c\,\hat{\mathbf{z}}$ | (6j) | Mg II |

## References


[1] J. Schefer, P. Fischer, W. Hälg, F. Stucki, L. Schlapbach, J. J. Didisheim, K. Yvon, and A. F. Andresen, *New structure results for hydrides and deuterides of the hydrogen storage material $Mg_2Ni$*, J. Less-Common Met. **74**, 65–73 (1980), doi:10.1016/0022-5088(80)90074-0.

[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.


## Found in


[1] P. Villars, *$Mg_2Ni$ Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) Springer Materials.


## First cited in


M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017