# $Al_3Ni_2$ ($D5_{13}$) Structure: A3B2_hP5_164_ad_d-001

This structure previously used the label(s) `A3B2_hP5_164_ad_d`. Calls to these addresses will be redirected here.

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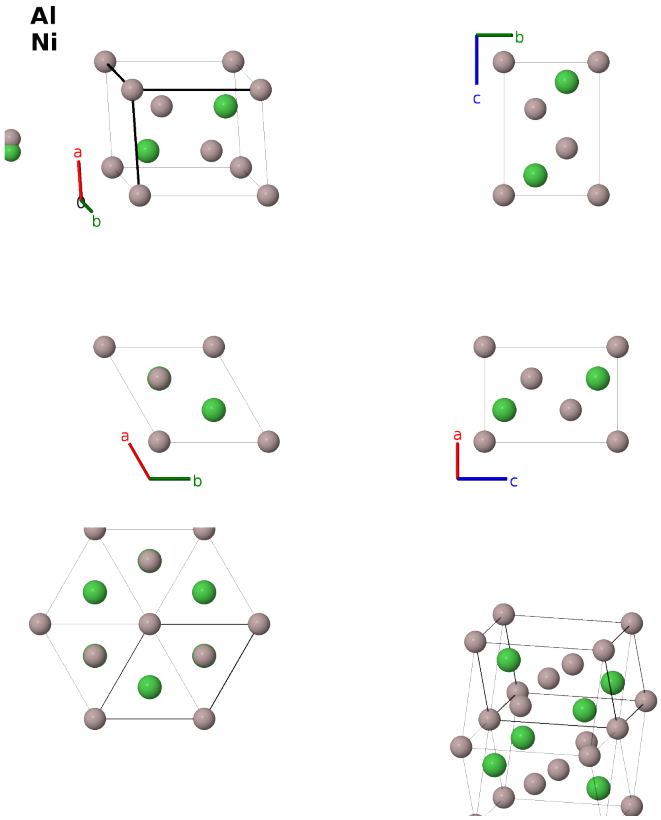
https://aflow.org/prototype-encyclopedia/EUFT

https://aflow.org/prototype-encyclopedia/A3B2_hP5_164_ad_d-001

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|---|---|
| **Prototype** | $Al_3Ni_2$ |
| **AFLOW prototype label** | A3B2_hP5_164_ad_d-001 |
| ***Strukturbericht* designation** | $D5_{13}$ |
| **ICSD** | 107937 |
| **CCDC** | 1665612 |
| **Pearson symbol** | hP5 |
| **Space group number** | 164 |
| **Space group symbol** | $P\bar{3}m1$ |

**AFLOW prototype command** `aflow --proto=A3B2_hP5_164_ad_d-001 --params=`$a, c/a, z_2, z_3$

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**Other compounds with this structure**

$Al_3Cu_2$, $Al_3In_2$, $Al_3Pd_2$, $Al_3Pt_2$, $Al_3Tc_2$, $Ga_3Pt_2$, $In_3Al_2$, $In_3Pd_2$, $In_3Pt_2$, $Mg_3Sb_2$, $\beta'$-$Ga_3Ni_2$, $\delta'$-$In_3Ni_2$

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- Either the three Al atoms or Al (1a) and the Ni atoms form a trigonal omega ($C6$) structure. Using the choices of internal parameters for $Al_3Ni_2$, this can be viewed as a five-layer close-packed unit cell with stacking ABCBCA.
- $Al_3Ni_2$ is isostructural with $La_2O_3$ ($D5_2$) and $Ce_2O_2S$. We use this structure for the binary intermetallics, $D5_2$ for the binary oxides and related structures, and $Ce_2O_2S$ for the ternary structures.

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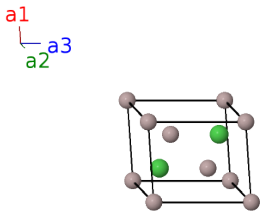
**Trigonal (Hexagonal) primitive vectors**

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

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (1a) | Al I |
| $\mathbf{B_2}$ | = | $\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (2d) | Al II |
| $\mathbf{B_3}$ | = | $\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$ | (2d) | Al II |
| $\mathbf{B_4}$ | = | $\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (2d) | Ni I |
| $\mathbf{B_5}$ | = | $\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (2d) | Ni I |

**References**


[1] A. J. Bradley and A. Taylor, *The crystal structures of $Ni_2Al_3$ and $NiAl_3$*, Philosophical Magazine **23**, 1049–1067 (1937), doi:10.1080/14786443708561875.


**Found in**


[1] P. Villars, K. Cenzual, J. Daams, R. Gladyshevskii, O. Shcherban, V. Dubenskyy, N. Melnichenko-Koblyuk, O. Pavlyuk, I. Savysyuk, S. Stoyko, and L. Sysa, *Structure Types. Part 6: Space Groups (166) R-3m - (160) R3m · $Ni_2Al_3$* (2008). Landolt-Börnstein - Group III Condensed Matter 43A6 (Springer-Verlag Berlin Heidelberg).


**First cited in**


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