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

This structure originally had the label `A3B2_hP5_164_ad_d`. Calls to that address will be redirected here.

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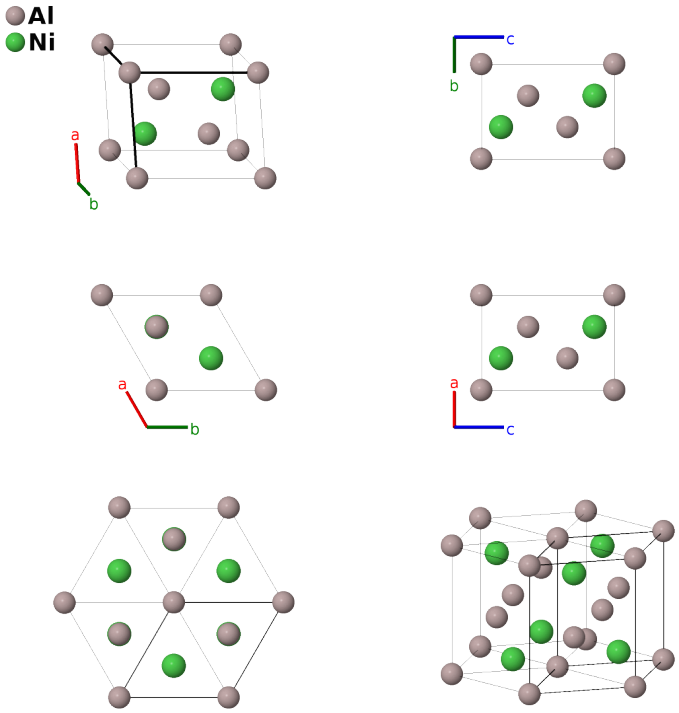
https://aflow.org/p/EUFT

https://aflow.org/p/A3B2_hP5_164_ad_d-001



Prototype	Al_3Ni_2
AFLOW prototype label	A3B2_hP5_164_ad_d-001
***Strukturbericht* designation**	$D5_{13}$
ICSD	107937
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=`$a, c/a, z_2, z_3$

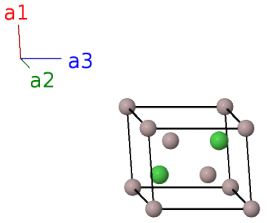
Other compounds with this structure

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, β'-Ga_3Ni_2, δ'-In_3Ni_2

- 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.

Trigonal (Hexagonal) primitive vectors

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



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).