$YNiAl_4$ Structure: A4BC_oC24_63_acf_c_c-002

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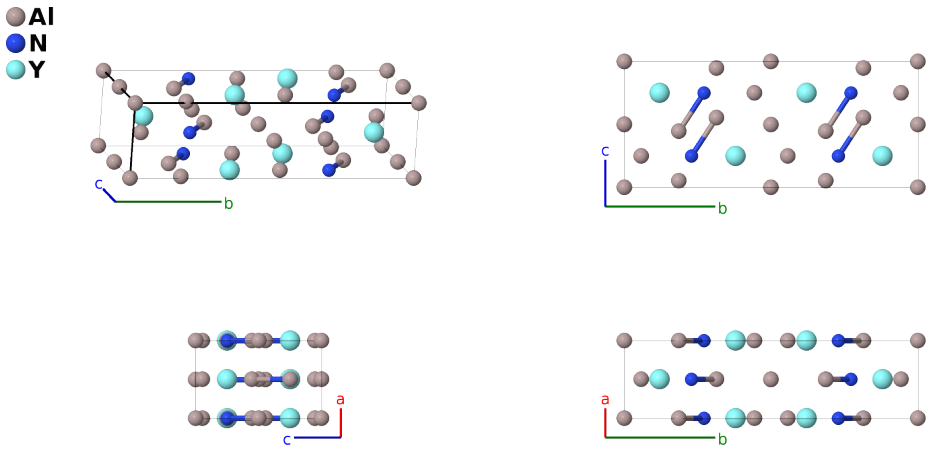
https://aflow.org/p/ULYP

https://aflow.org/p/A4BC_oC24_63_acf_c_c-002



Prototype	Al_4NiY
AFLOW prototype label	A4BC_oC24_63_acf_c_c-002
ICSD	58077
Pearson symbol	oC24
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=A4BC_oC24_63_acf_c_c-002 --params=`$a, b/a, c/a, y_2, y_3, y_4, y_5, z_5$

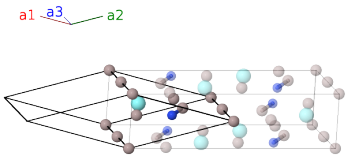
Other compounds with this structure

$CdPdIn_4$, $CeNiAl_4$, $DyNiAl_4$, $EuAuIn_4$, $EuIrAl_4$, $EuIrIn_4$, $EuPtIr_4$, $GdNiAl_4$, $LaPtIr_4$, $NdNiAl_4$, $SrPtIr_4$, $YPtIr_4$, $YbPtIr_4$

- We use the data from (Rykhal, 1972) as quoted by (Shin, 2008). This includes a shift in the origin so that the Al-I atoms is at the (4a) Wyckoff position rather than the (4b) position used by (Rykhal, 1972).

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Al II
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Al II
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	N I
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	N I
$\mathbf{B_7}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Y I
$\mathbf{B_8}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Y I
$\mathbf{B_9}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8f)	Al III
$\mathbf{B_{10}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Al III
$\mathbf{B_{11}}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Al III
$\mathbf{B_{12}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8f)	Al III

References

[1] D. Shin, W. J. Golumbfskie, E. R. Ryba, and Z.-K. Liu, *First-principles study of Al–Ni–Y ternary compounds for crystal structure validation*, J. Alloys Compd. **462**, 262–266 (2008), doi:10.1016/j.jallcom.2007.08.010.

[2] R. M. Rykhal, O. S. Zarechnyuk, and Y. P. Yarmolyuk, *Crystal structure of the compounds $YNiAl_4 and YNiAl_2$.*, Sov. Phys. Crystallograph. **17**, 521–524 (1972).