ZrNiAl Structure: ABC_hP9_189_f_bc_g-003

This structure originally had the label `ABC_hP9_189_g_ad_f`. Calls to that address will be redirected here.

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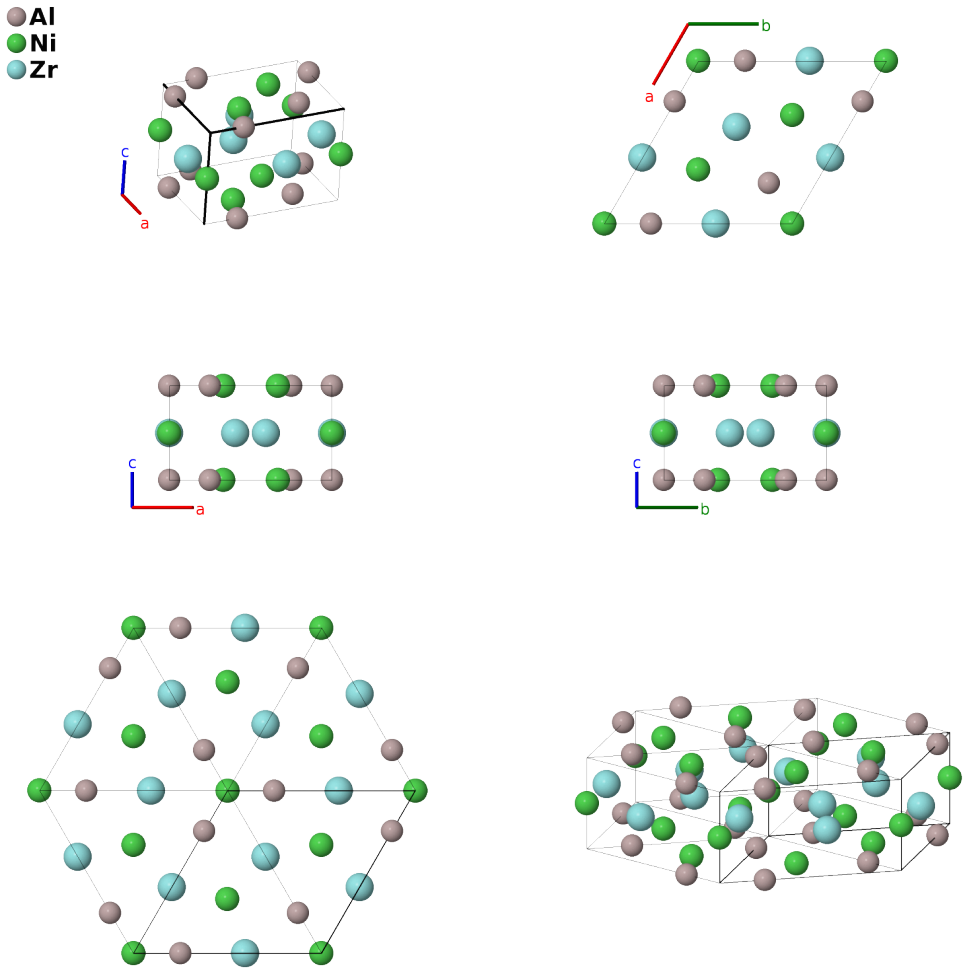
https://aflow.org/p/0T4U

https://aflow.org/p/ABC_hP9_189_f_bc_g-003



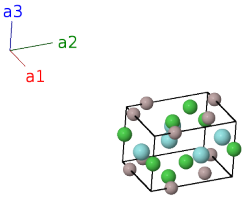
Prototype	AlNiZr
AFLOW prototype label	ABC_hP9_189_f_bc_g-003
ICSD	152131
Pearson symbol	hP9
Space group number	189
Space group symbol	$P\bar{6}2m$
AFLOW prototype command	`aflow --proto=ABC_hP9_189_f_bc_g-003 --params=`$a, c/a, x_3, x_4$

Other compounds with this structure
AgAsCa, AgSiYb, AlCoPu, AlCuTm, AlNiTb, DyNiIn, DyNiSn, ErNiAl, FeCoAs, FeGaU, FeNiP, GaNiZr, GaPdSc, GdNiIn, GdNiSn, HoNiIn, RhSnZr, RuSiZr, ScIrP, TbNiIn, TiFeP, ZrRuAs, BSi_2Ni_6

- This a the ternary form of the Fe_2P structure. While (Shved, 2019) placed the nickel atoms on the (1a) and (2d) sites, as in Fe_2P, we have shifted to origin by $\frac{1}{2}c\hat{z}$ to place them on the (1b) and (2c) sites. Otherwise the structures are nearly identical.
- (Shved, 2019) found evidence of 6-10% mixing between the Ni-II (2d) and Al (3g) sites.
- (Shved, 2019) has no entry in the ICSD, so we reference the ZrNiAl entry from (Zumdick, 1999).

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
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Ni I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Ni II
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Ni II
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3f)	Al I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_2$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3f)	Al I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}}$	(3f)	Al I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Zr I
$\mathbf{B_8}$	=	$x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Zr I
$\mathbf{B_9}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Zr I

References

[1] O. Shved, L. P. Salamakha, S. Mudry, O. Sologub, P. F. Rogl, and E. Bauer, *Zr-based nickel aluminides: crystal structure and electronic properties*, J. Alloys Compd. p. 153326 (2019), doi:10.1016/j.jallcom.2019.153326. In press.

[2] M. F. Zumdick, R.-D. Hoffmann, and R. Pöttgen, *The Intermetallic Zirconium Compounds ZrNiAl, ZrRhSn, and ZrPtGa - Structural Distortions and Metal-Metal Bonding in Fe_2P Related Compounds*, Z. Naturforsch. B **54**, 45–53 (1999), doi:10.1515/znb-1999-0111.