Zr_7Ni_{10} Structure: A10B7_oC68_64_f2g_adef-001

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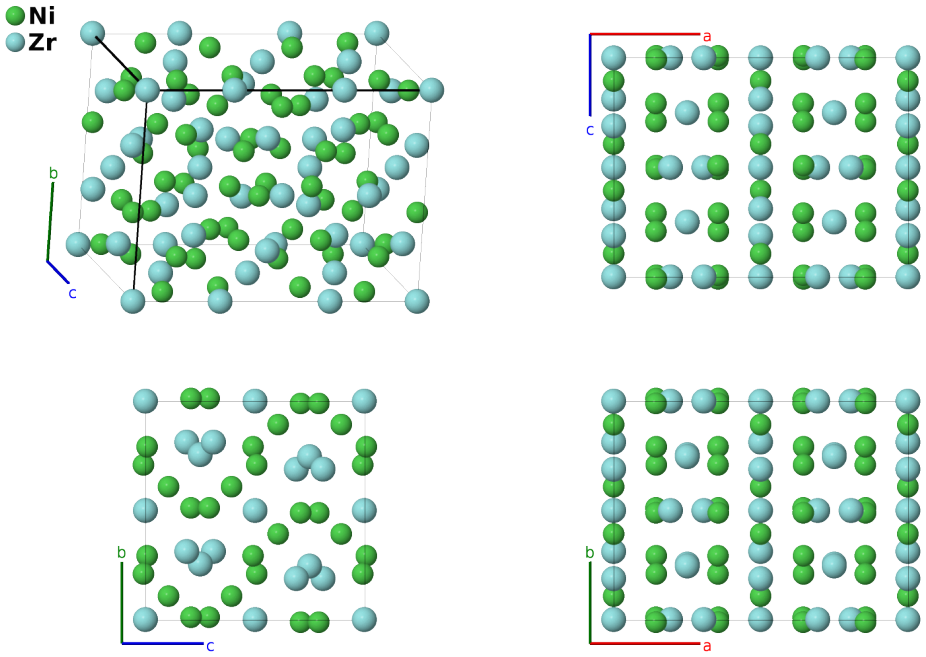
https://aflow.org/p/7BKZ

https://aflow.org/p/A10B7_oC68_64_f2g_adef-001



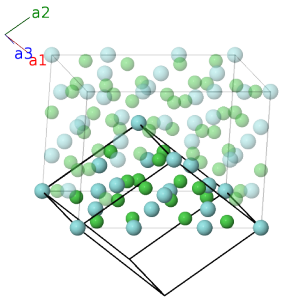
Prototype	$Ni_{10}Zr_7$
AFLOW prototype label	A10B7_oC68_64_f2g_adef-001
ICSD	240191
Pearson symbol	oC68
Space group number	64
Space group symbol	*Cmce*
AFLOW prototype command	`aflow --proto=A10B7_oC68_64_f2g_adef-001 --params=`$a, b/a, c/a, x_2, y_3, y_4, z_4, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

Other compounds with this structure
Hf_7Ni_{10}

- (Kirkpatrick, 1962) originally placed this structure in space group *Aba*2 #41, and early structure compilations such as (Pearson, 1967) quote this structure. (Joubert, 1977) showed that the structure has an inversion site and placed the system in space group *Cmca* #64.

Base-centered Orthorhombic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Zr I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Zr I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}}$	(8d)	Zr II
$\mathbf{B_4}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Zr II
$\mathbf{B_5}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}}$	(8d)	Zr II
$\mathbf{B_6}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Zr II
$\mathbf{B_7}$	=	$-\left(y_3 - \frac{1}{4}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	Zr III
$\mathbf{B_8}$	=	$\left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8e)	Zr III
$\mathbf{B_9}$	=	$\left(y_3 + \frac{3}{4}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8e)	Zr III
$\mathbf{B_{10}}$	=	$-\left(y_3 - \frac{3}{4}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	Zr III
$\mathbf{B_{11}}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8f)	Ni I
$\mathbf{B_{12}}$	=	$\left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Ni I
$\mathbf{B_{13}}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Ni I
$\mathbf{B_{14}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8f)	Ni I
$\mathbf{B_{15}}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8f)	Zr IV
$\mathbf{B_{16}}$	=	$\left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Zr IV
$\mathbf{B_{17}}$	=	$-\left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Zr IV
$\mathbf{B_{18}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8f)	Zr IV
$\mathbf{B_{19}}$	=	$(x_6 - y_6)\,\mathbf{a}_1 + (x_6 + y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(16g)	Ni II
$\mathbf{B_{20}}$	=	$\left(-x_6 + y_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_6 + y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	Ni II
$\mathbf{B_{21}}$	=	$-\left(x_6 + y_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_6 + y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16g)	Ni II

$$\mathbf{B_{22}} = (x_6 + y_6)\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3 = a x_6\,\hat{\mathbf{x}} - b y_6\,\hat{\mathbf{y}} - c z_6\,\hat{\mathbf{z}} \quad (16g) \quad \text{Ni II}$$

$$\mathbf{B_{23}} = -(x_6 - y_6)\,\mathbf{a}_1 - (x_6 + y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3 = -a x_6\,\hat{\mathbf{x}} - b y_6\,\hat{\mathbf{y}} - c z_6\,\hat{\mathbf{z}} \quad (16g) \quad \text{Ni II}$$

$$\mathbf{B_{24}} = \left(x_6 - y_6 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_6 + y_6 + \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_6 - \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_6 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + b y_6\,\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16g) \quad \text{Ni II}$$

$$\mathbf{B_{25}} = \left(x_6 + y_6 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_6 - y_6 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_6 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b y_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16g) \quad \text{Ni II}$$

$$\mathbf{B_{26}} = -(x_6 + y_6)\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = -a x_6\,\hat{\mathbf{x}} + b y_6\,\hat{\mathbf{y}} + c z_6\,\hat{\mathbf{z}} \quad (16g) \quad \text{Ni II}$$

$$\mathbf{B_{27}} = (x_7 - y_7)\,\mathbf{a}_1 + (x_7 + y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = a x_7\,\hat{\mathbf{x}} + b y_7\,\hat{\mathbf{y}} + c z_7\,\hat{\mathbf{z}} \quad (16g) \quad \text{Ni III}$$

$$\mathbf{B_{28}} = \left(-x_7 + y_7 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(x_7 + y_7 - \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_7 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - b y_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16g) \quad \text{Ni III}$$

$$\mathbf{B_{29}} = -\left(x_7 + y_7 - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(-x_7 + y_7 + \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_7 - \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_7 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b y_7\,\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16g) \quad \text{Ni III}$$

$$\mathbf{B_{30}} = (x_7 + y_7)\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = a x_7\,\hat{\mathbf{x}} - b y_7\,\hat{\mathbf{y}} - c z_7\,\hat{\mathbf{z}} \quad (16g) \quad \text{Ni III}$$

$$\mathbf{B_{31}} = -(x_7 - y_7)\,\mathbf{a}_1 - (x_7 + y_7)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = -a x_7\,\hat{\mathbf{x}} - b y_7\,\hat{\mathbf{y}} - c z_7\,\hat{\mathbf{z}} \quad (16g) \quad \text{Ni III}$$

$$\mathbf{B_{32}} = \left(x_7 - y_7 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_7 + y_7 + \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_7 - \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_7 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + b y_7\,\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16g) \quad \text{Ni III}$$

$$\mathbf{B_{33}} = \left(x_7 + y_7 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_7 - y_7 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_7 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b y_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16g) \quad \text{Ni III}$$

$$\mathbf{B_{34}} = -(x_7 + y_7)\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = -a x_7\,\hat{\mathbf{x}} + b y_7\,\hat{\mathbf{y}} + c z_7\,\hat{\mathbf{z}} \quad (16g) \quad \text{Ni III}$$

References

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[2] M. E. Kirkpatrick, J. F. Smith, and W. L. Larsen, *Structures of the intermediate phases $Ni_{10}Zr_7$ and $Ni_{10}Hf_7$*, Acta Cryst. **15**, 894–903 (1962), doi:10.1107/S0365110X62002339.

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