

Zr₇Ni₁₀ Structure:

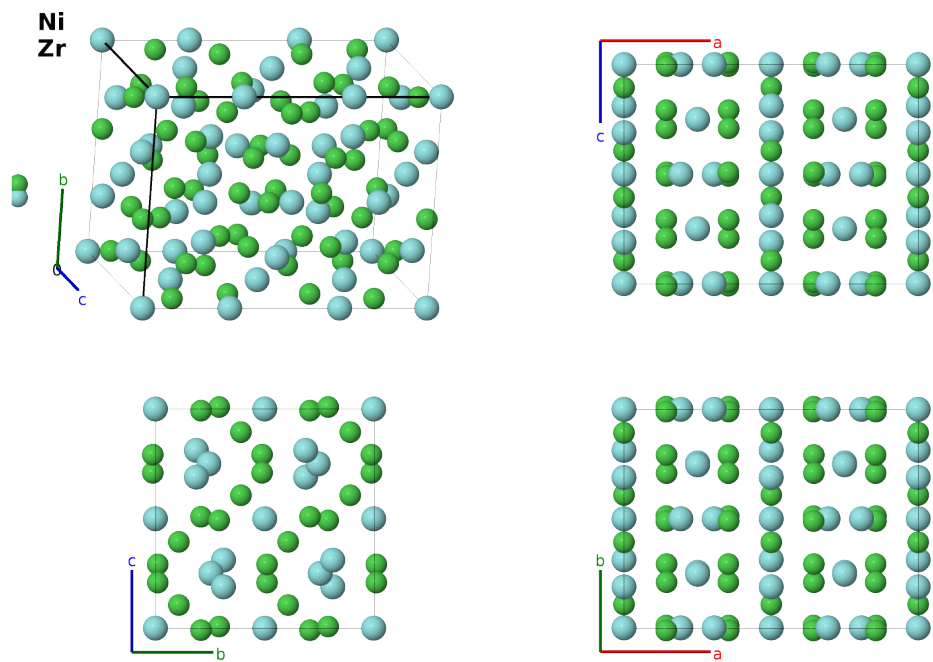
A10B7_oC68_64_f2g_adeF-001

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<https://afLOW.org/prototype-encyclopedia/7BKZ>

https://afLOW.org/prototype-encyclopedia/A10B7_oC68_64_f2g_adeF-001



Prototype	Ni ₁₀ Zr ₇
AFLOW prototype label	A10B7_oC68_64_f2g_adeF-001
ICSD	240191
CCDC	1710940
Pearson symbol	oC68
Space group number	64
Space group symbol	<i>Cmce</i>
AFLOW prototype command	<code>afLOW --proto=A10B7_oC68_64_f2g_adeF-001</code> <code>--params=a, b/a, c/a, x₂, y₃, y₄, z₄, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇</code>

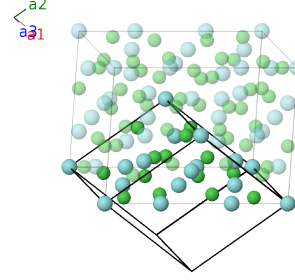
Other compounds with this structure

Hf₇Ni₁₀

- (Kirkpatrick, 1962) originally placed this structure in space group *Aba2* #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

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



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

$$\begin{aligned}
\mathbf{B}_{21} &= \begin{matrix} -\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 \end{matrix} = -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) & \text{Ni II} \\
\mathbf{B}_{22} &= \begin{matrix} (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 - \\ z_6 \mathbf{a}_3 \end{matrix} = ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (16g) & \text{Ni II} \\
\mathbf{B}_{23} &= \begin{matrix} -(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 - \\ z_6 \mathbf{a}_3 \end{matrix} = -ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (16g) & \text{Ni II} \\
\mathbf{B}_{24} &= \begin{matrix} \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 \end{matrix} = 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) & \text{Ni II} \\
\mathbf{B}_{25} &= \begin{matrix} \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 \end{matrix} = 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) & \text{Ni II} \\
\mathbf{B}_{26} &= \begin{matrix} -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + \\ z_6 \mathbf{a}_3 \end{matrix} = -ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (16g) & \text{Ni II} \\
\mathbf{B}_{27} &= \begin{matrix} (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + \\ z_7 \mathbf{a}_3 \end{matrix} = ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (16g) & \text{Ni III} \\
\mathbf{B}_{28} &= \begin{matrix} \left(-x_7 + y_7 + \frac{1}{2}\right) \mathbf{a}_1 - \\ \left(x_7 + y_7 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 \end{matrix} = -a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (16g) & \text{Ni III} \\
\mathbf{B}_{29} &= \begin{matrix} -\left(x_7 + y_7 - \frac{1}{2}\right) \mathbf{a}_1 + \\ \left(-x_7 + y_7 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 \end{matrix} = -a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} & (16g) & \text{Ni III} \\
\mathbf{B}_{30} &= \begin{matrix} (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 - \\ z_7 \mathbf{a}_3 \end{matrix} = ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (16g) & \text{Ni III} \\
\mathbf{B}_{31} &= \begin{matrix} -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 - \\ z_7 \mathbf{a}_3 \end{matrix} = -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (16g) & \text{Ni III} \\
\mathbf{B}_{32} &= \begin{matrix} \left(x_7 - y_7 + \frac{1}{2}\right) \mathbf{a}_1 + \\ \left(x_7 + y_7 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 \end{matrix} = a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} & (16g) & \text{Ni III} \\
\mathbf{B}_{33} &= \begin{matrix} \left(x_7 + y_7 + \frac{1}{2}\right) \mathbf{a}_1 + \\ \left(x_7 - y_7 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 \end{matrix} = a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (16g) & \text{Ni III} \\
\mathbf{B}_{34} &= \begin{matrix} -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 + \\ z_7 \mathbf{a}_3 \end{matrix} = -ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (16g) & \text{Ni III}
\end{aligned}$$

References

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Found in

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