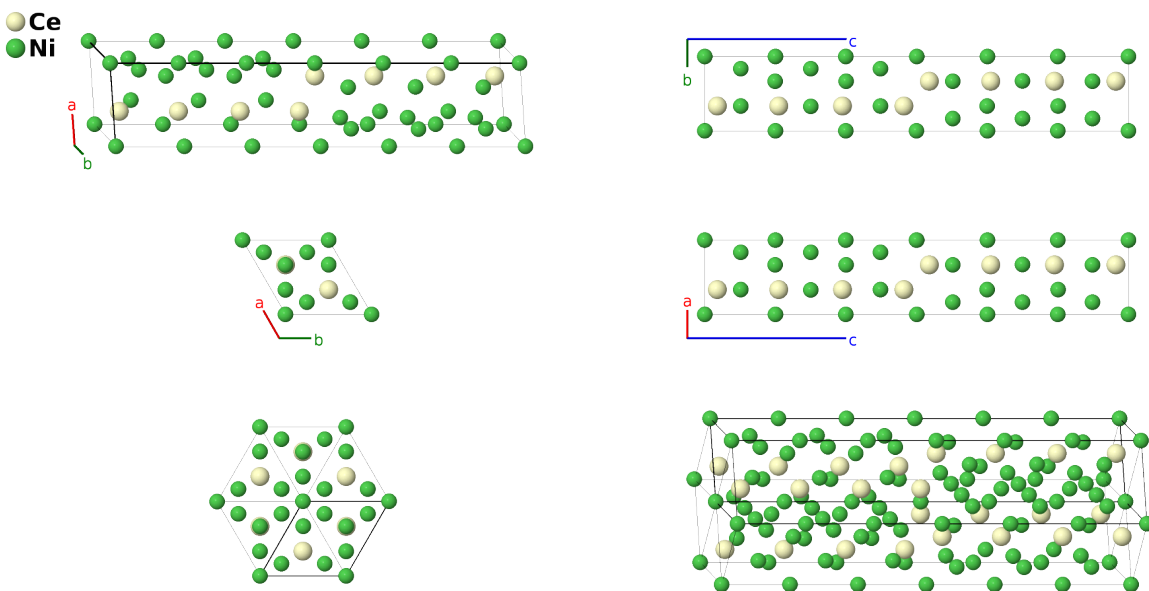


Ce₂Ni₇ Structure: A2B7_hP36_194_2f_aefhk-001

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<https://afLOW.org/p/A0TL>

https://afLOW.org/p/A2B7_hP36_194_2f_aefhk-001



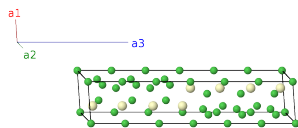
Prototype	Ce ₂ Ni ₇
AFLOW prototype label	A2B7_hP36_194_2f_aefhk-001
ICSD	102233
Pearson symbol	hP36
Space group number	194
Space group symbol	<i>P</i> 6 ₃ / <i>mmc</i>
AFLOW prototype command	<code>afLOW --proto=A2B7_hP36_194_2f_aefhk-001 --params=a, c/a, z₂, z₃, z₄, z₅, x₆, x₇, z₇</code>

Other compounds with this structure

Ce₂Ni₇, Dy₂Ni₇, Er₂Ni₇, Gd₂Co₇, La₂Ni₇, La₂Rh₇, Nd₂Ni₇, Sm₂Co₇, Th₂Fe₇, Th₂Ni₇, Y₂Ni₇

Hexagonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$=$	0	$=$	0	(2a) Ni I
\mathbf{B}_2	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(2a) Ni I
\mathbf{B}_3	$=$	$z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(4e) Ni II
\mathbf{B}_4	$=$	$(z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e) Ni II
\mathbf{B}_5	$=$	$-z_2 \mathbf{a}_3$	$=$	$-cz_2 \hat{\mathbf{z}}$	(4e) Ni II
\mathbf{B}_6	$=$	$-(z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e) Ni II
\mathbf{B}_7	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4f) Ce I
\mathbf{B}_8	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f) Ce I
\mathbf{B}_9	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4f) Ce I
\mathbf{B}_{10}	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f) Ce I
\mathbf{B}_{11}	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4f) Ce II
\mathbf{B}_{12}	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f) Ce II
\mathbf{B}_{13}	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4f) Ce II
\mathbf{B}_{14}	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f) Ce II
\mathbf{B}_{15}	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4f) Ni III
\mathbf{B}_{16}	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f) Ni III
\mathbf{B}_{17}	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4f) Ni III
\mathbf{B}_{18}	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f) Ni III
\mathbf{B}_{19}	$=$	$x_6 \mathbf{a}_1 + 2x_6 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{2} ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} ax_6 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h) Ni IV
\mathbf{B}_{20}	$=$	$-2x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2} ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} ax_6 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h) Ni IV
\mathbf{B}_{21}	$=$	$x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\sqrt{3} ax_6 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(6h) Ni IV
\mathbf{B}_{22}	$=$	$-x_6 \mathbf{a}_1 - 2x_6 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2} ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} ax_6 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h) Ni IV
\mathbf{B}_{23}	$=$	$2x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{2} ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} ax_6 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h) Ni IV
\mathbf{B}_{24}	$=$	$-x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\sqrt{3} ax_6 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(6h) Ni IV
\mathbf{B}_{25}	$=$	$x_7 \mathbf{a}_1 + 2x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{3}{2} ax_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(12k) Ni V
\mathbf{B}_{26}	$=$	$-2x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-\frac{3}{2} ax_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(12k) Ni V
\mathbf{B}_{27}	$=$	$x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-\sqrt{3} ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(12k) Ni V
\mathbf{B}_{28}	$=$	$-x_7 \mathbf{a}_1 - 2x_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{3}{2} ax_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k) Ni V
\mathbf{B}_{29}	$=$	$2x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{2} ax_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k) Ni V
\mathbf{B}_{30}	$=$	$-x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\sqrt{3} ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(12k) Ni V
\mathbf{B}_{31}	$=$	$2x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$\frac{3}{2} ax_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(12k) Ni V
\mathbf{B}_{32}	$=$	$-x_7 \mathbf{a}_1 - 2x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-\frac{3}{2} ax_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2} ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(12k) Ni V
\mathbf{B}_{33}	$=$	$-x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$\sqrt{3} ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(12k) Ni V
\mathbf{B}_{34}	$=$	$-2x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{3}{2} ax_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} ax_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(12k) Ni V
\mathbf{B}_{35}	$=$	$x_7 \mathbf{a}_1 + 2x_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{2} ax_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2} ax_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(12k) Ni V
\mathbf{B}_{36}	$=$	$x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-\sqrt{3} ax_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(12k) Ni V

References

- [1] D. T. Cromer and A. C. Larson, *The Crystal Structure of Ce₂Ni₇*, Acta Cryst. **12**, 855–859 (1959), doi:10.1107/S0365110X59002468.