

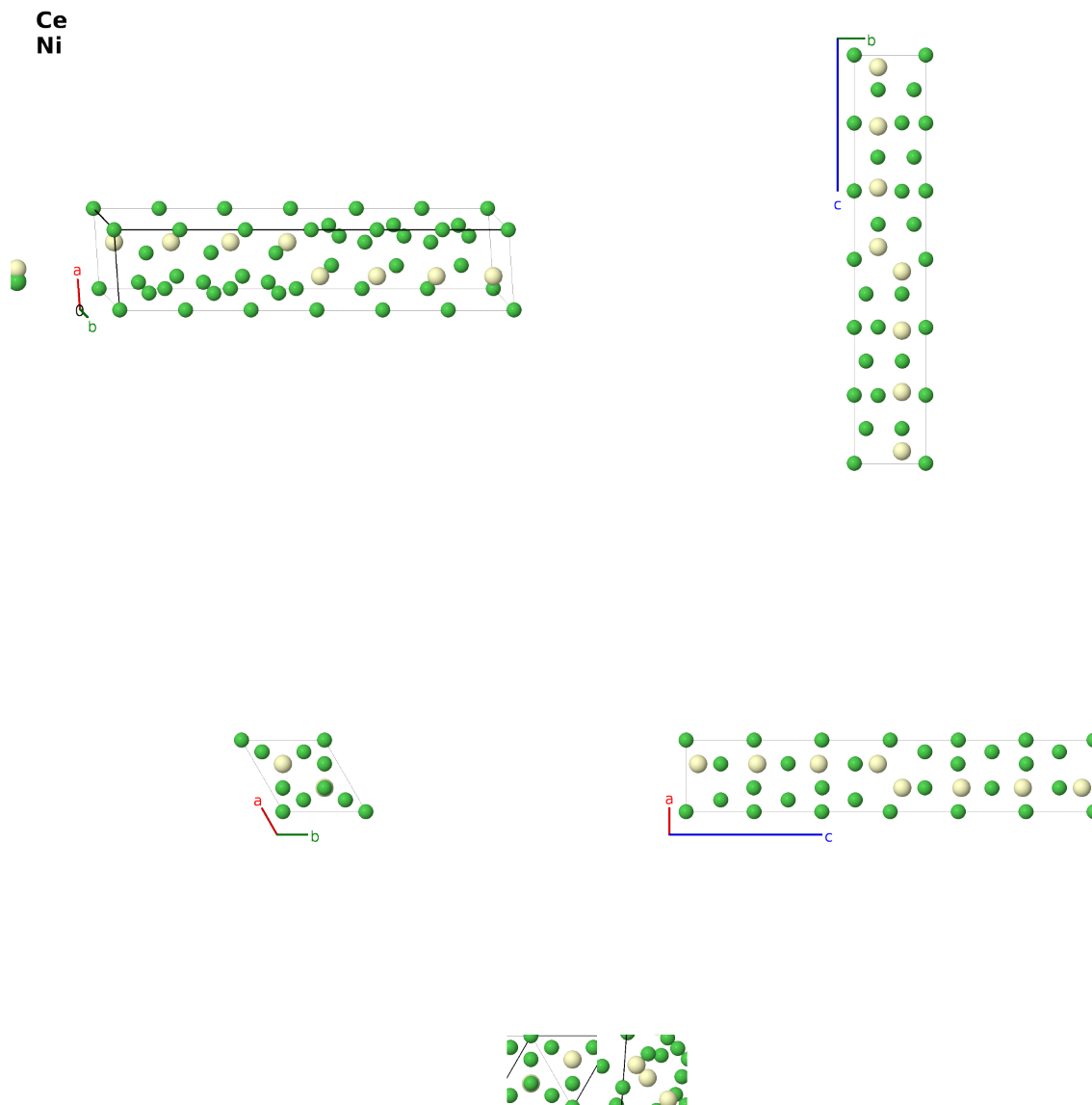
Ce₂Ni₇ Structure: A2B7_hP36_194_2f_aefhk-001

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<https://aflow.org/prototype-encyclopedia/A0TL>

https://aflow.org/prototype-encyclopedia/A2B7_hP36_194_2f_aefhk-001



Prototype	Ce ₂ Ni ₇
AFLOW prototype label	A2B7_hP36_194_2f_aefhk-001
ICSD	102233
CCDC	1660220

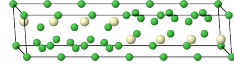
Pearson symbol	hP36
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	aflow --proto=A2B7_hP36_194_2f_aefhk-001 --params= $a, c/a, z_2, z_3, z_4, z_5, x_6, x_7, z_7$

Other compounds with this structure

Ce₂Co₇, Dy₂Ni₇, Er₂Ni₇, Eu₂Pt₇, Gd₂Co₇, Gd₂Ni₇, La₂Co₇, La₂Ir₇, La₂Ni₇, La₂Rh₇, Nd₂Co₇, Nd₂Ni₇, Pr₂Co₇, Pr₂Ni₇, Sc₂Ni₇, Sm₂Co₇, Sm₂Ni₇, Tb₂Ni₇, Th₂Co₇, 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
$\mathbf{B}_{28}$	$= -x_7 \mathbf{a}_1 - 2x_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12k)	Ni V
$\mathbf{B}_{29}$	$= 2x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{3}{2}ax_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12k)	Ni V
$\mathbf{B}_{30}$	$= -x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\sqrt{3}ax_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{34}$	$= -2x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12k)	Ni V
$\mathbf{B}_{35}$	$= x_7 \mathbf{a}_1 + 2x_7 \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{3}{2}ax_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12k)	Ni V
$\mathbf{B}_{36}$	$= x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\sqrt{3}ax_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12k)	Ni V

References

- [1] D. T. Cromer and A. C. Larson, *The Crystal Structure of Ce_2Ni_7* , Acta Cryst. **12**, 855–859 (1959), doi:10.1107/S0365110X59002468.

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