$Ce_3Ni_6Si_2$ Structure: A3B6C2_cI44_229_e_h_c-001

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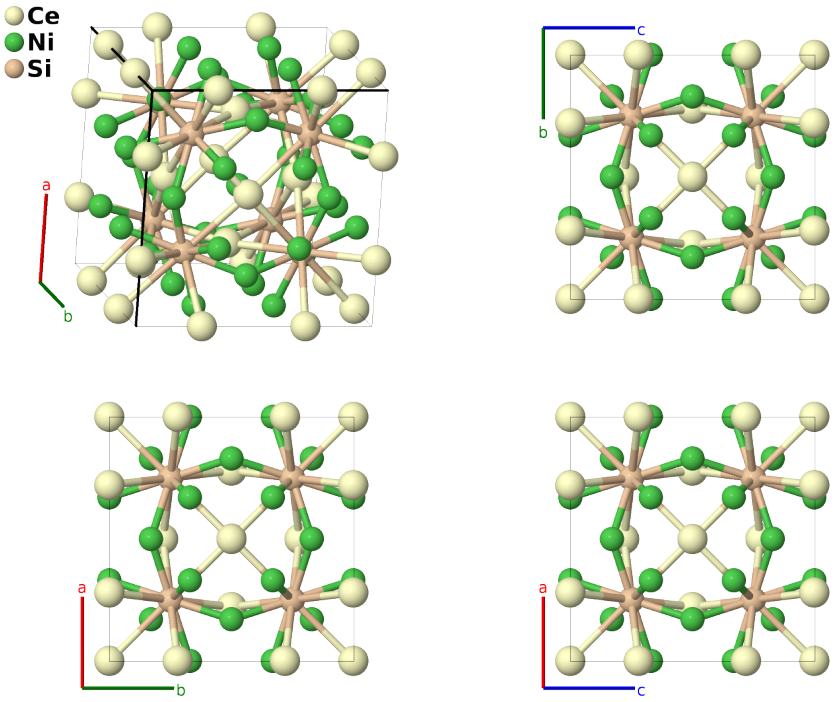
https://aflow.org/p/BC5E

https://aflow.org/p/A3B6C2_cI44_229_e_h_c-001



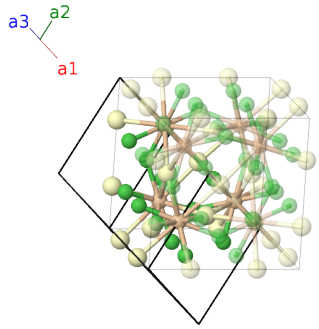
Prototype	$Ce_3Ni_6Si_2$
AFLOW prototype label	A3B6C2_cI44_229_e_h_c-001
ICSD	25622
Pearson symbol	cI44
Space group number	229
Space group symbol	$Im\bar{3}m$
AFLOW prototype command	`aflow --proto=A3B6C2_cI44_229_e_h_c-001 --params=`a, x_2, y_3

Other compounds with this structure

$Dy_3Ni_6Si_2$, $Er_3Ni_6Al_2$, $Er_3Ni_6Si_2$, $Eu_3Ni_6Si_2$, $Gd_3Ni_6Si_2$, $Ho_3Ni_6Si_2$, $Lu_3Ni_6Si_2$, $Nd_3Ni_6Si_2$, $Pr_3Ni_6Si_2$, $Sm_3Ni_6Si_2$, $Tb_3Ni_6Si_2$, $Tm_3Ni_6Si_2$, $U_3Ni_6Ge_2$, $U_3Ni_6Si_2$, $Yb_3Ni_6Si_2$

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Si I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Si I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Si I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Si I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}$	(12e)	Ce I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}$	(12e)	Ce I
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{y}}$	(12e)	Ce I
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{y}}$	(12e)	Ce I
$\mathbf{B_9}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{z}}$	(12e)	Ce I
$\mathbf{B_{10}}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{z}}$	(12e)	Ce I
$\mathbf{B_{11}}$	=	$2y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(24h)	Ni I
$\mathbf{B_{12}}$	=	$y_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(24h)	Ni I
$\mathbf{B_{13}}$	=	$-y_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}}$	(24h)	Ni I
$\mathbf{B_{14}}$	=	$-2y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}}$	(24h)	Ni I
$\mathbf{B_{15}}$	=	$y_3\,\mathbf{a}_1 + 2y_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{z}}$	(24h)	Ni I
$\mathbf{B_{16}}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{z}}$	(24h)	Ni I
$\mathbf{B_{17}}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{z}}$	(24h)	Ni I
$\mathbf{B_{18}}$	=	$-y_3\,\mathbf{a}_1 - 2y_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{z}}$	(24h)	Ni I
$\mathbf{B_{19}}$	=	$y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + 2y_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}}$	(24h)	Ni I
$\mathbf{B_{20}}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2$	=	$-ay_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}}$	(24h)	Ni I
$\mathbf{B_{21}}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2$	=	$ay_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}}$	(24h)	Ni I
$\mathbf{B_{22}}$	=	$-y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - 2y_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}}$	(24h)	Ni I

References

[1] E. I. Hladyschewskyj, P. I. Krypiakewytsch, and O. I. Bodak, *Die Kristallstruktur von $Ce_3Ni_6Si_2$ und verwandten Verbindungen*, Z. Anorganische und Allgemeine Chemie **344**, 95–101 (1966), doi:10.1002/zaac.19663440113.