Ni_3Ti ($D0_{24}$) Structure: A3B_hP16_194_gh_ac-001

This structure previously used the label(s) `A3B_hP16_194_gh_ac`. Calls to these addresses will be redirected here.

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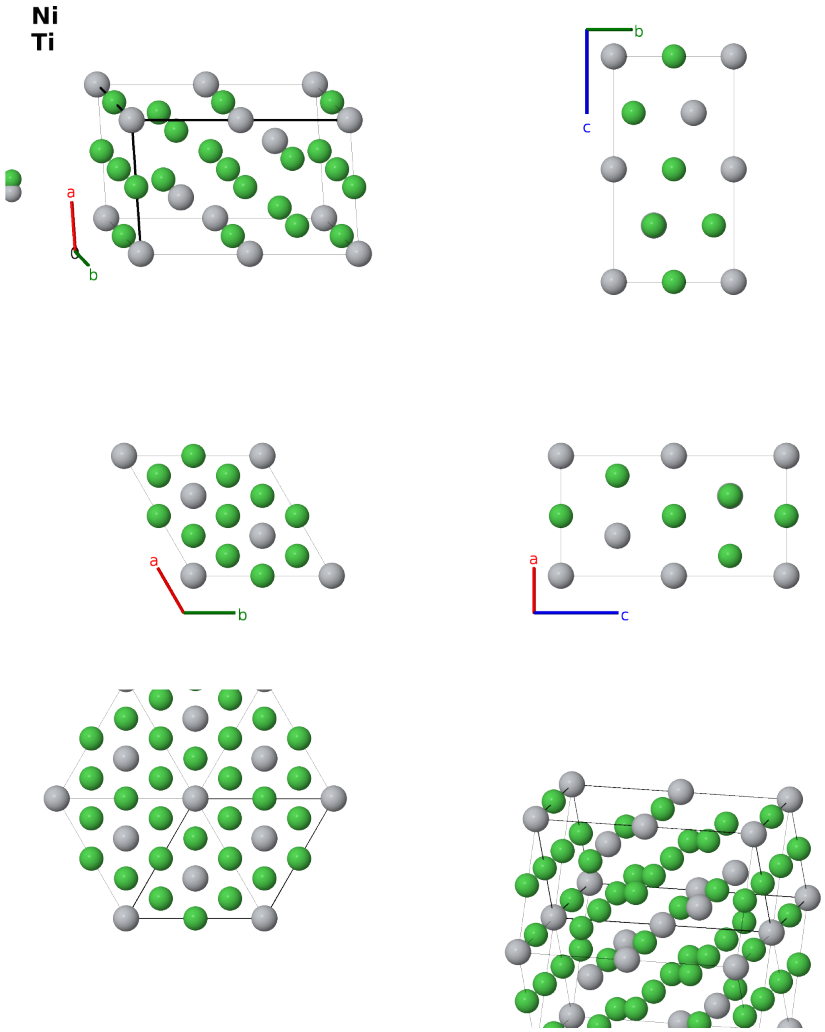
https://aflow.org/prototype-encyclopedia/7D2A

https://aflow.org/prototype-encyclopedia/A3B_hP16_194_gh_ac-001



Prototype	Ni_3Ti
AFLOW prototype label	A3B_hP16_194_gh_ac-001
***Strukturbericht* designation**	$D0_{24}$
ICSD	30216

CCDC	1604588
Pearson symbol	hP16
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=A3B_hP16_194_gh_ac-001 --params=`$a, c/a, x_4$

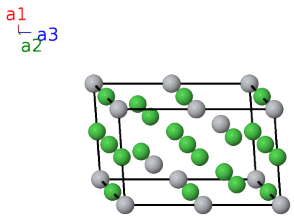
Other compounds with this structure

Al_3Dy, Al_3Ru, Co_3Ti, Ni_3Ti, Pd_3Hf, Pd_3Np, Pd_3Th, Pd_3Ti, Pd_3Zr, Pt_3Hf, Pt_3Zr

- The internal coordinate x_4 was not determined in any reference we could find. We follow (Villars, 2016) and the ICSD and set $x_4 = -1/6$, which places the niobium atoms in line with the Ti atoms in the $z = 1/4$ and $z = 3/4$ planes. This is not required by symmetry, and it is likely that the actual value of x_4 will be close, but not equal to, $-1/6$.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ti I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Ti I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Ti II
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Ti II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(6g)	Ni I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(6g)	Ni I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(6g)	Ni I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Ni I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Ni I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Ni I
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1 + 2x_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Ni II
$\mathbf{B_{12}}$	=	$-2x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Ni II
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Ni II
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 - 2x_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Ni II
$\mathbf{B_{15}}$	=	$2x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Ni II

$\mathbf{B_{16}} = -x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3 = \sqrt{3}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ (6h) Ni II

References

[1] F. Laves and H. J. Wallbaum, *Die Kristallstruktur von Ni_3Ti und Si_2Ti (Zwei neue Typen.)*, Z. Krystallogr. **101**, 78–93 (1939), doi:10.1524/zkri.1939.101.1.78.

Found in

[1] P. Villars, ed., *PAULING FILE in: Inorganic Solid Phases* (SpringerMaterials (online database), Heidelberg, 2016).

First cited in

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