

NiTi₂ Structure:

AB2_cF96_227_e_cf-001

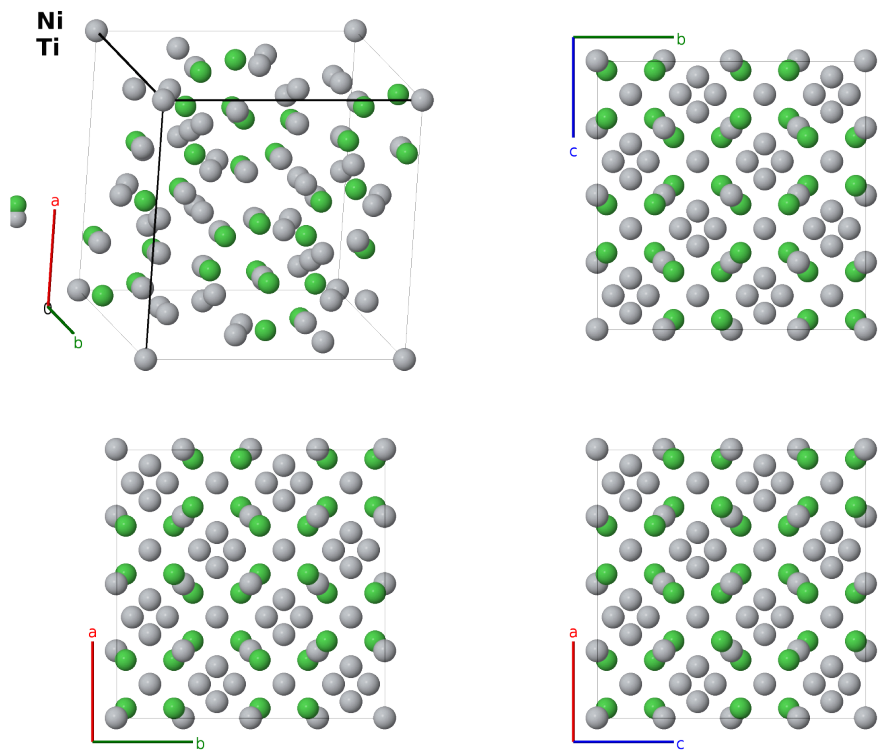
This structure previously used the label(s) **AB2_cF96_227_e_cf**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/AB2_cF96_227_e_cf-001



Prototype	NiTi ₂
AFLOW prototype label	AB2_cF96_227_e_cf-001
ICSD	105420
CCDC	1663308
Pearson symbol	cF96
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	<code>aflow --proto=AB2_cF96_227_e_cf-001</code> <code>--params=a, x_2, x_3</code>

Other compounds with this structure

CoHf₂, CoTi₂, CoZr₂, FeTi₂, FeZr₂, IrHf₂, IrSc₂, IrZr₂, MnHf₂, NbCr₂, NiSc₂, OsHf₂, PdSc₂, PtHf₂, RhHf₂

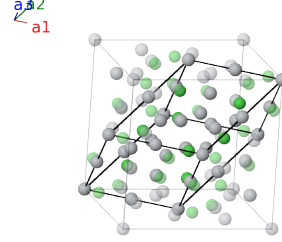
- We have used the fact that all vectors of the form $(0, \pm a/2, \pm a/2)$, $(\pm a/2, 0, \pm a/2)$, and $(\pm a/2, \pm a/2, 0)$ are primitive vectors of the face-centered cubic lattice to simplify the positions of some atoms in both lattice and Cartesian coordinates.

Face-centered Cubic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(16c) Ti I
$\mathbf{B}_2$	$=$	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}}$	(16c) Ti I
$\mathbf{B}_3$	$=$	$\frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16c) Ti I
$\mathbf{B}_4$	$=$	$\frac{1}{2}\mathbf{a}_1$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16c) Ti I
$\mathbf{B}_5$	$=$	$x_2\mathbf{a}_1 + x_2\mathbf{a}_2 + x_2\mathbf{a}_3$	$=$	$ax_2\hat{\mathbf{x}} + ax_2\hat{\mathbf{y}} + ax_2\hat{\mathbf{z}}$	(32e) Ni I
$\mathbf{B}_6$	$=$	$x_2\mathbf{a}_1 + x_2\mathbf{a}_2 - (3x_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{4})\hat{\mathbf{x}} - a(x_2 - \frac{1}{4})\hat{\mathbf{y}} + ax_2\hat{\mathbf{z}}$	(32e) Ni I
$\mathbf{B}_7$	$=$	$x_2\mathbf{a}_1 - (3x_2 - \frac{1}{2})\mathbf{a}_2 + x_2\mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{4})\hat{\mathbf{x}} + ax_2\hat{\mathbf{y}} - a(x_2 - \frac{1}{4})\hat{\mathbf{z}}$	(32e) Ni I
$\mathbf{B}_8$	$=$	$-(3x_2 - \frac{1}{2})\mathbf{a}_1 + x_2\mathbf{a}_2 + x_2\mathbf{a}_3$	$=$	$ax_2\hat{\mathbf{x}} - a(x_2 - \frac{1}{4})\hat{\mathbf{y}} - a(x_2 - \frac{1}{4})\hat{\mathbf{z}}$	(32e) Ni I
$\mathbf{B}_9$	$=$	$-x_2\mathbf{a}_1 - x_2\mathbf{a}_2 + (3x_2 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{4})\hat{\mathbf{x}} + a(x_2 + \frac{1}{4})\hat{\mathbf{y}} - ax_2\hat{\mathbf{z}}$	(32e) Ni I
$\mathbf{B}_{10}$	$=$	$-x_2\mathbf{a}_1 - x_2\mathbf{a}_2 - x_2\mathbf{a}_3$	$=$	$-ax_2\hat{\mathbf{x}} - ax_2\hat{\mathbf{y}} - ax_2\hat{\mathbf{z}}$	(32e) Ni I
$\mathbf{B}_{11}$	$=$	$-x_2\mathbf{a}_1 + (3x_2 + \frac{1}{2})\mathbf{a}_2 - x_2\mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{4})\hat{\mathbf{x}} - ax_2\hat{\mathbf{y}} + a(x_2 + \frac{1}{4})\hat{\mathbf{z}}$	(32e) Ni I
$\mathbf{B}_{12}$	$=$	$(3x_2 + \frac{1}{2})\mathbf{a}_1 - x_2\mathbf{a}_2 - x_2\mathbf{a}_3$	$=$	$-ax_2\hat{\mathbf{x}} + a(x_2 + \frac{1}{4})\hat{\mathbf{y}} + a(x_2 + \frac{1}{4})\hat{\mathbf{z}}$	(32e) Ni I
$\mathbf{B}_{13}$	$=$	$-(x_3 - \frac{1}{4})\mathbf{a}_1 + x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(48f) Ti II
$\mathbf{B}_{14}$	$=$	$x_3\mathbf{a}_1 - (x_3 - \frac{1}{4})\mathbf{a}_2 - (x_3 - \frac{1}{4})\mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(48f) Ti II
$\mathbf{B}_{15}$	$=$	$x_3\mathbf{a}_1 - (x_3 - \frac{1}{4})\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + ax_3\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(48f) Ti II
$\mathbf{B}_{16}$	$=$	$-(x_3 - \frac{1}{4})\mathbf{a}_1 + x_3\mathbf{a}_2 - (x_3 - \frac{1}{4})\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} - a(x_3 - \frac{1}{4})\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(48f) Ti II
$\mathbf{B}_{17}$	$=$	$x_3\mathbf{a}_1 + x_3\mathbf{a}_2 - (x_3 - \frac{1}{4})\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + ax_3\hat{\mathbf{z}}$	(48f) Ti II
$\mathbf{B}_{18}$	$=$	$-(x_3 - \frac{1}{4})\mathbf{a}_1 - (x_3 - \frac{1}{4})\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} - a(x_3 - \frac{1}{4})\hat{\mathbf{z}}$	(48f) Ti II
$\mathbf{B}_{19}$	$=$	$(x_3 + \frac{3}{4})\mathbf{a}_1 - x_3\mathbf{a}_2 + (x_3 + \frac{3}{4})\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} + a(x_3 + \frac{3}{4})\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(48f) Ti II
$\mathbf{B}_{20}$	$=$	$-x_3\mathbf{a}_1 + (x_3 + \frac{3}{4})\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} - ax_3\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(48f) Ti II
$\mathbf{B}_{21}$	$=$	$-x_3\mathbf{a}_1 + (x_3 + \frac{3}{4})\mathbf{a}_2 + (x_3 + \frac{3}{4})\mathbf{a}_3$	$=$	$a(x_3 + \frac{3}{4})\hat{\mathbf{x}} + \frac{3}{8}a\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(48f) Ti II

$$\mathbf{B}_{22} = \left(x_3 + \frac{3}{4}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3 = -ax_3 \hat{\mathbf{x}} + \frac{3}{8}a \hat{\mathbf{y}} + \frac{3}{8}a \hat{\mathbf{z}} \quad (48f) \quad \text{Ti II}$$

$$\mathbf{B}_{23} = -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(x_3 + \frac{3}{4}\right) \mathbf{a}_3 = \frac{3}{8}a \hat{\mathbf{x}} + \frac{3}{8}a \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}} \quad (48f) \quad \text{Ti II}$$

$$\mathbf{B}_{24} = \left(x_3 + \frac{3}{4}\right) \mathbf{a}_1 + \left(x_3 + \frac{3}{4}\right) \mathbf{a}_2 - x_3 \mathbf{a}_3 = \frac{3}{8}a \hat{\mathbf{x}} + \frac{3}{8}a \hat{\mathbf{y}} + a \left(x_3 + \frac{3}{4}\right) \hat{\mathbf{z}} \quad (48f) \quad \text{Ti II}$$

References

- [1] G. A. Yurko, J. W. Barton, and J. G. Parr, *The crystal structure of Ti_2Ni* , Acta Cryst. **12**, 909–911 (1959), doi:10.1107/S0365110X59002559.

Found in

- [1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.

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