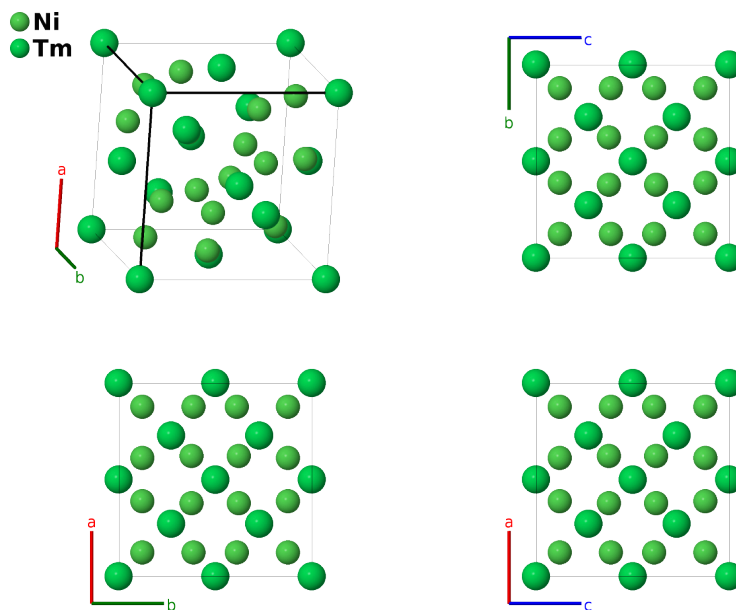


# Intermediate Temperature TmNi<sub>2</sub> Structure: A2B\_cP24\_215\_ei\_ace-001

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<https://aflow.org/p/X751>

[https://aflow.org/p/A2B\\_cP24\\_215\\_ei\\_ace-001](https://aflow.org/p/A2B_cP24_215_ei_ace-001)

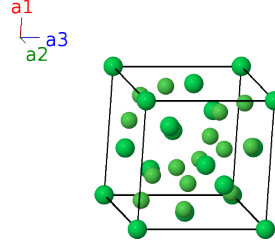


<b>Prototype</b>	Ni <sub>2</sub> Tm
<b>AFLOW prototype label</b>	A2B_cP24_215_ei_ace-001
<b>ICSD</b>	none
<b>Pearson symbol</b>	cP24
<b>Space group number</b>	215
<b>Space group symbol</b>	$P\bar{4}3m$
<b>AFLOW prototype command</b>	<code>aflow --proto=A2B_cP24_215_ei_ace-001 --params=a, x<sub>3</sub>, x<sub>4</sub>, x<sub>5</sub>, z<sub>5</sub></code>

- TmNi<sub>2</sub> is found in three forms (Deutz, 1989):
  - A low temperature face-centered cubic structure at room temperature and below,
  - a simple cubic structure (this structure) near 700°, and
  - the C15 cubic Laves structure for higher temperatures.
- The data for this structure was taken at 700°. (Deutz, 1989) did not provide the lattice constant, so we estimated it from the size of the low temperature structure at 300K.

## Simple Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$0$	$=$	$0$	(1a)	Tm I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(3c)	Tm II
$\mathbf{B}_3$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(3c)	Tm II
$\mathbf{B}_4$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(3c)	Tm II
$\mathbf{B}_5$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(4e)	Ni I
$\mathbf{B}_6$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(4e)	Ni I
$\mathbf{B}_7$	$-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(4e)	Ni I
$\mathbf{B}_8$	$x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(4e)	Ni I
$\mathbf{B}_9$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(4e)	Tm III
$\mathbf{B}_{10}$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(4e)	Tm III
$\mathbf{B}_{11}$	$-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(4e)	Tm III
$\mathbf{B}_{12}$	$x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(4e)	Tm III
$\mathbf{B}_{13}$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + az_5 \hat{\mathbf{z}}$	(12i)	Ni II
$\mathbf{B}_{14}$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + az_5 \hat{\mathbf{z}}$	(12i)	Ni II
$\mathbf{B}_{15}$	$-x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}}$	(12i)	Ni II
$\mathbf{B}_{16}$	$x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}}$	(12i)	Ni II
$\mathbf{B}_{17}$	$z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$az_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(12i)	Ni II
$\mathbf{B}_{18}$	$z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$az_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(12i)	Ni II
$\mathbf{B}_{19}$	$-z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-az_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(12i)	Ni II
$\mathbf{B}_{20}$	$-z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-az_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(12i)	Ni II
$\mathbf{B}_{21}$	$x_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(12i)	Ni II
$\mathbf{B}_{22}$	$-x_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(12i)	Ni II
$\mathbf{B}_{23}$	$x_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(12i)	Ni II
$\mathbf{B}_{24}$	$-x_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(12i)	Ni II

## References

- [1] A. F. Deutz, R. B. Helmholtz, A. C. Moleman, D. B. D. Mooij, and K. H. J. Buschow, *Superstructure in the intermetallic compound  $TmNi_2$* , J. Less-Common Met. **153**, 259–266 (1989), doi:10.1016/0022-5088(89)90120-3.