

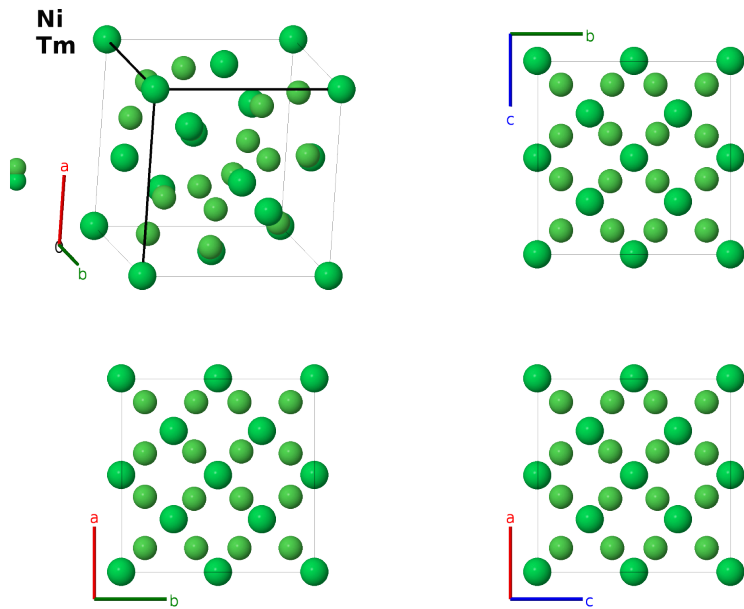
Intermediate Temperature TmNi₂ Structure: A2B_cP24_215_ei_ace-001

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<https://aflow.org/prototype-encyclopedia/X751>

https://aflow.org/prototype-encyclopedia/A2B_cP24_215_ei_ace-001



Prototype	Ni ₂ Tm
AFLOW prototype label	A2B_cP24_215_ei_ace-001
Pearson symbol	cP24
Space group number	215
Space group symbol	$P\bar{4}3m$
AFLOW prototype command	<code>aflow --proto=A2B_cP24_215_ei_ace-001 --params=a, x₃, x₄, x₅, z₅</code>

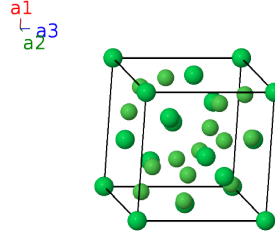
- TmNi₂ is found in three forms (Deutz, 1989):
 - A low temperature face-centered cubic structure at room temperature and below,
 - a simple cubic structure (this structure) near 700°, and
 - the C15 cubic Laves structure for higher temperatures.
- The data for this structure was taken at 700°. (Deutz, 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

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



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. Helmholdt, 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.

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