

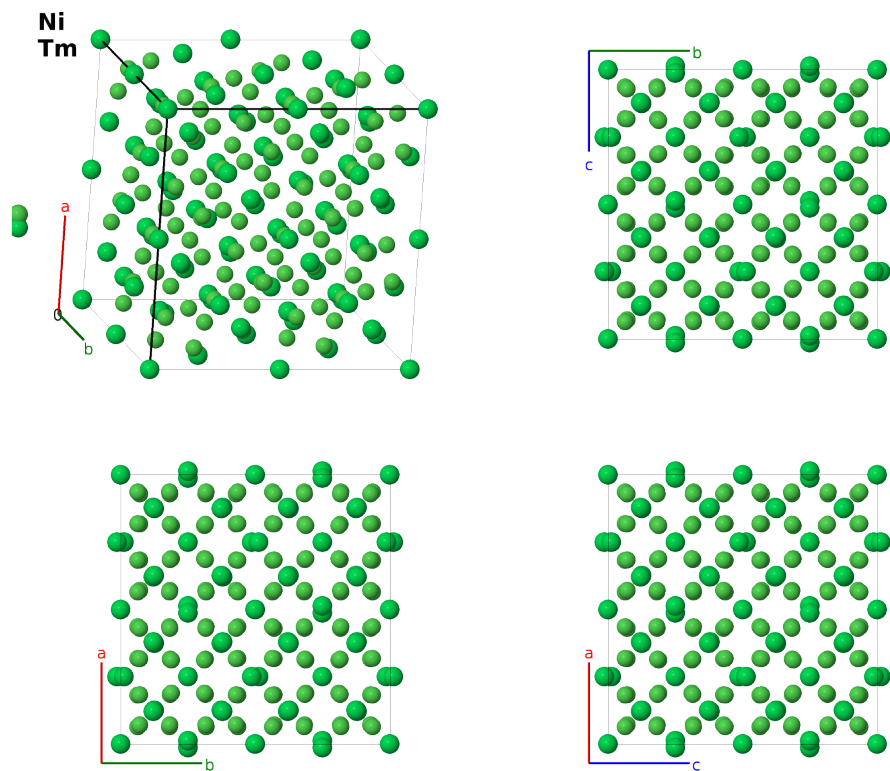
Low Temperature TmNi₂ Structure: A2B_cF192_216_2e2h_ab2eg-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/5WAR>

https://aflow.org/prototype-encyclopedia/A2B_cF192_216_2e2h_ab2eg-001

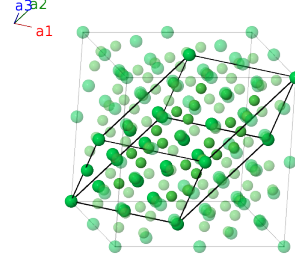


Prototype	Ni ₂ Tm
AFLOW prototype label	A2B_cF192_216_2e2h_ab2eg-001
ICSD	105432
CCDC	1663319
Pearson symbol	cF192
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	<code>aflow --proto=A2B_cF192_216_2e2h_ab2eg-001</code> <code>--params=a, x₃, x₄, x₅, x₆, x₇, x₈, z₈, x₉, z₉</code>

- TmNi₂ is found in three forms (Deutz, 1989):
 - A low temperature face-centered cubic structure (this structure) at room temperature and below,
 - a simple cubic structure near 700°, and
 - the C15 cubic Laves structure for higher temperatures.
- The data for this structure was taken at 4.2K.

Face-centered Cubic primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} \\
 \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}} \\
 \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}
 \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(4a) Tm I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(4b) Tm II
$\mathbf{B}_3$	=	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16e) Ni I
$\mathbf{B}_4$	=	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - 3x_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16e) Ni I
$\mathbf{B}_5$	=	$x_3 \mathbf{a}_1 - 3x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16e) Ni I
$\mathbf{B}_6$	=	$-3x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16e) Ni I
$\mathbf{B}_7$	=	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(16e) Ni II
$\mathbf{B}_8$	=	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - 3x_4 \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(16e) Ni II
$\mathbf{B}_9$	=	$x_4 \mathbf{a}_1 - 3x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(16e) Ni II
$\mathbf{B}_{10}$	=	$-3x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(16e) Ni II
$\mathbf{B}_{11}$	=	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(16e) Tm III
$\mathbf{B}_{12}$	=	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - 3x_5 \mathbf{a}_3$	=	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(16e) Tm III
$\mathbf{B}_{13}$	=	$x_5 \mathbf{a}_1 - 3x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$-ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(16e) Tm III
$\mathbf{B}_{14}$	=	$-3x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(16e) Tm III
$\mathbf{B}_{15}$	=	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	=	$ax_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + ax_6 \hat{\mathbf{z}}$	(16e) Tm IV
$\mathbf{B}_{16}$	=	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - 3x_6 \mathbf{a}_3$	=	$-ax_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + ax_6 \hat{\mathbf{z}}$	(16e) Tm IV
$\mathbf{B}_{17}$	=	$x_6 \mathbf{a}_1 - 3x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	=	$-ax_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}}$	(16e) Tm IV
$\mathbf{B}_{18}$	=	$-3x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	=	$ax_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}}$	(16e) Tm IV
$\mathbf{B}_{19}$	=	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$ax_7 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g) Tm V
$\mathbf{B}_{20}$	=	$x_7 \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 - (x_7 - \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g) Tm V
$\mathbf{B}_{21}$	=	$x_7 \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 + x_7 \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g) Tm V
$\mathbf{B}_{22}$	=	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + x_7 \mathbf{a}_2 - (x_7 - \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g) Tm V

$$\begin{aligned}
\mathbf{B}_{23} &= x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - \left(x_7 - \frac{1}{2}\right) \mathbf{a}_3 &= \frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}} &(24g) &\text{Tm V} \\
\mathbf{B}_{24} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right) \mathbf{a}_2 + x_7 \mathbf{a}_3 &= \frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{z}} &(24g) &\text{Tm V} \\
\mathbf{B}_{25} &= z_8 \mathbf{a}_1 + z_8 \mathbf{a}_2 + (2x_8 - z_8) \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + az_8 \hat{\mathbf{z}} &(48h) &\text{Ni III} \\
\mathbf{B}_{26} &= z_8 \mathbf{a}_1 + z_8 \mathbf{a}_2 - (2x_8 + z_8) \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + az_8 \hat{\mathbf{z}} &(48h) &\text{Ni III} \\
\mathbf{B}_{27} &= (2x_8 - z_8) \mathbf{a}_1 - (2x_8 + z_8) \mathbf{a}_2 + z_8 \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - az_8 \hat{\mathbf{z}} &(48h) &\text{Ni III} \\
\mathbf{B}_{28} &= -(2x_8 + z_8) \mathbf{a}_1 + (2x_8 - z_8) \mathbf{a}_2 + z_8 \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - az_8 \hat{\mathbf{z}} &(48h) &\text{Ni III} \\
\mathbf{B}_{29} &= (2x_8 - z_8) \mathbf{a}_1 + z_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= az_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}} &(48h) &\text{Ni III} \\
\mathbf{B}_{30} &= -(2x_8 + z_8) \mathbf{a}_1 + z_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= az_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}} &(48h) &\text{Ni III} \\
\mathbf{B}_{31} &= z_8 \mathbf{a}_1 + (2x_8 - z_8) \mathbf{a}_2 - (2x_8 + z_8) \mathbf{a}_3 &= -az_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}} &(48h) &\text{Ni III} \\
\mathbf{B}_{32} &= z_8 \mathbf{a}_1 - (2x_8 + z_8) \mathbf{a}_2 + (2x_8 - z_8) \mathbf{a}_3 &= -az_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}} &(48h) &\text{Ni III} \\
\mathbf{B}_{33} &= z_8 \mathbf{a}_1 + (2x_8 - z_8) \mathbf{a}_2 + z_8 \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} + az_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}} &(48h) &\text{Ni III} \\
\mathbf{B}_{34} &= z_8 \mathbf{a}_1 - (2x_8 + z_8) \mathbf{a}_2 + z_8 \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} + az_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}} &(48h) &\text{Ni III} \\
\mathbf{B}_{35} &= -(2x_8 + z_8) \mathbf{a}_1 + z_8 \mathbf{a}_2 + (2x_8 - z_8) \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} - az_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}} &(48h) &\text{Ni III} \\
\mathbf{B}_{36} &= (2x_8 - z_8) \mathbf{a}_1 + z_8 \mathbf{a}_2 - (2x_8 + z_8) \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} - az_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}} &(48h) &\text{Ni III} \\
\mathbf{B}_{37} &= z_9 \mathbf{a}_1 + z_9 \mathbf{a}_2 + (2x_9 - z_9) \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} + az_9 \hat{\mathbf{z}} &(48h) &\text{Ni IV} \\
\mathbf{B}_{38} &= z_9 \mathbf{a}_1 + z_9 \mathbf{a}_2 - (2x_9 + z_9) \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} + az_9 \hat{\mathbf{z}} &(48h) &\text{Ni IV} \\
\mathbf{B}_{39} &= (2x_9 - z_9) \mathbf{a}_1 - (2x_9 + z_9) \mathbf{a}_2 + z_9 \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} - az_9 \hat{\mathbf{z}} &(48h) &\text{Ni IV} \\
\mathbf{B}_{40} &= -(2x_9 + z_9) \mathbf{a}_1 + (2x_9 - z_9) \mathbf{a}_2 + z_9 \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} - az_9 \hat{\mathbf{z}} &(48h) &\text{Ni IV} \\
\mathbf{B}_{41} &= (2x_9 - z_9) \mathbf{a}_1 + z_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 &= az_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} + ax_9 \hat{\mathbf{z}} &(48h) &\text{Ni IV} \\
\mathbf{B}_{42} &= -(2x_9 + z_9) \mathbf{a}_1 + z_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 &= az_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} - ax_9 \hat{\mathbf{z}} &(48h) &\text{Ni IV} \\
\mathbf{B}_{43} &= z_9 \mathbf{a}_1 + (2x_9 - z_9) \mathbf{a}_2 - (2x_9 + z_9) \mathbf{a}_3 &= -az_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} + ax_9 \hat{\mathbf{z}} &(48h) &\text{Ni IV} \\
\mathbf{B}_{44} &= z_9 \mathbf{a}_1 - (2x_9 + z_9) \mathbf{a}_2 + (2x_9 - z_9) \mathbf{a}_3 &= -az_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} - ax_9 \hat{\mathbf{z}} &(48h) &\text{Ni IV} \\
\mathbf{B}_{45} &= z_9 \mathbf{a}_1 + (2x_9 - z_9) \mathbf{a}_2 + z_9 \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} + az_9 \hat{\mathbf{y}} + ax_9 \hat{\mathbf{z}} &(48h) &\text{Ni IV} \\
\mathbf{B}_{46} &= z_9 \mathbf{a}_1 - (2x_9 + z_9) \mathbf{a}_2 + z_9 \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} + az_9 \hat{\mathbf{y}} - ax_9 \hat{\mathbf{z}} &(48h) &\text{Ni IV} \\
\mathbf{B}_{47} &= -(2x_9 + z_9) \mathbf{a}_1 + z_9 \mathbf{a}_2 + (2x_9 - z_9) \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} - az_9 \hat{\mathbf{y}} - ax_9 \hat{\mathbf{z}} &(48h) &\text{Ni IV} \\
\mathbf{B}_{48} &= (2x_9 - z_9) \mathbf{a}_1 + z_9 \mathbf{a}_2 - (2x_9 + z_9) \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} - az_9 \hat{\mathbf{y}} + ax_9 \hat{\mathbf{z}} &(48h) &\text{Ni IV}
\end{aligned}$$

References

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- [1] A. Jain, S. Ping, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, and K. A. Persson, *Commentary: The Materials Project: A materials genome approach to accelerating materials innovation*, APL Materials **1**, 011002 (2013), doi:10.1063/1.4812323.

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