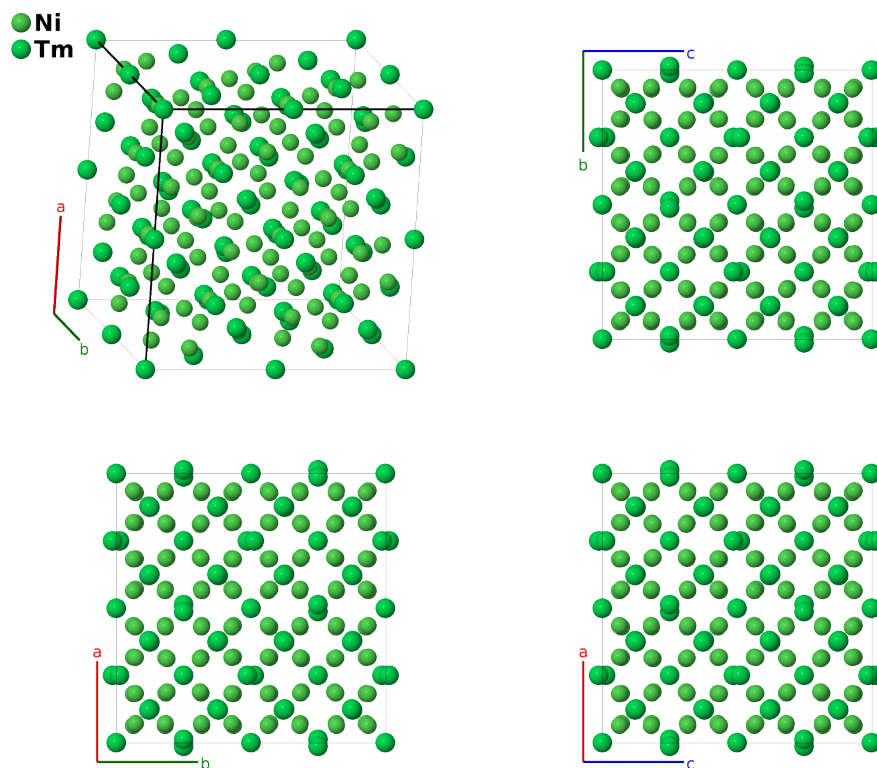


Low Temperature TmNi₂ Structure: A2B_cF192_216_2e2h_ab2eg-001

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<https://aflow.org/p/5WAR>

https://aflow.org/p/A2B_cF192_216_2e2h_ab2eg-001



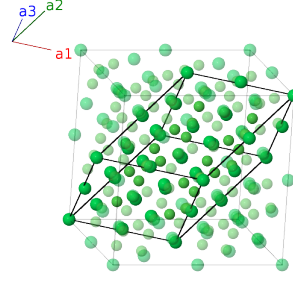
Prototype	Ni ₂ Tm
AFLOW prototype label	A2B_cF192_216_2e2h_ab2eg-001
ICSD	105432
Pearson symbol	cF192
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	<code>aflow --proto=A2B_cF192_216_2e2h_ab2eg-001 --params=a, x₃, x₄, x₅, x₆, x₇, x₈, z₈, x₉, z₉</code>

- 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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(4a)	Tm I
\mathbf{B}_2	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z}$	(4b)	Tm II
\mathbf{B}_3	$x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{x} + ax_3\hat{y} + ax_3\hat{z}$	(16e)	Ni I
\mathbf{B}_4	$x_3\mathbf{a}_1 + x_3\mathbf{a}_2 - 3x_3\mathbf{a}_3$	$=$	$-ax_3\hat{x} - ax_3\hat{y} + ax_3\hat{z}$	(16e)	Ni I
\mathbf{B}_5	$x_3\mathbf{a}_1 - 3x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$-ax_3\hat{x} + ax_3\hat{y} - ax_3\hat{z}$	(16e)	Ni I
\mathbf{B}_6	$-3x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{x} - ax_3\hat{y} - ax_3\hat{z}$	(16e)	Ni I
\mathbf{B}_7	$x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$ax_4\hat{x} + ax_4\hat{y} + ax_4\hat{z}$	(16e)	Ni II
\mathbf{B}_8	$x_4\mathbf{a}_1 + x_4\mathbf{a}_2 - 3x_4\mathbf{a}_3$	$=$	$-ax_4\hat{x} - ax_4\hat{y} + ax_4\hat{z}$	(16e)	Ni II
\mathbf{B}_9	$x_4\mathbf{a}_1 - 3x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$-ax_4\hat{x} + ax_4\hat{y} - ax_4\hat{z}$	(16e)	Ni II
\mathbf{B}_{10}	$-3x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$ax_4\hat{x} - ax_4\hat{y} - ax_4\hat{z}$	(16e)	Ni II
\mathbf{B}_{11}	$x_5\mathbf{a}_1 + x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$ax_5\hat{x} + ax_5\hat{y} + ax_5\hat{z}$	(16e)	Tm III
\mathbf{B}_{12}	$x_5\mathbf{a}_1 + x_5\mathbf{a}_2 - 3x_5\mathbf{a}_3$	$=$	$-ax_5\hat{x} - ax_5\hat{y} + ax_5\hat{z}$	(16e)	Tm III
\mathbf{B}_{13}	$x_5\mathbf{a}_1 - 3x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$-ax_5\hat{x} + ax_5\hat{y} - ax_5\hat{z}$	(16e)	Tm III
\mathbf{B}_{14}	$-3x_5\mathbf{a}_1 + x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$ax_5\hat{x} - ax_5\hat{y} - ax_5\hat{z}$	(16e)	Tm III
\mathbf{B}_{15}	$x_6\mathbf{a}_1 + x_6\mathbf{a}_2 + x_6\mathbf{a}_3$	$=$	$ax_6\hat{x} + ax_6\hat{y} + ax_6\hat{z}$	(16e)	Tm IV
\mathbf{B}_{16}	$x_6\mathbf{a}_1 + x_6\mathbf{a}_2 - 3x_6\mathbf{a}_3$	$=$	$-ax_6\hat{x} - ax_6\hat{y} + ax_6\hat{z}$	(16e)	Tm IV
\mathbf{B}_{17}	$x_6\mathbf{a}_1 - 3x_6\mathbf{a}_2 + x_6\mathbf{a}_3$	$=$	$-ax_6\hat{x} + ax_6\hat{y} - ax_6\hat{z}$	(16e)	Tm IV
\mathbf{B}_{18}	$-3x_6\mathbf{a}_1 + x_6\mathbf{a}_2 + x_6\mathbf{a}_3$	$=$	$ax_6\hat{x} - ax_6\hat{y} - ax_6\hat{z}$	(16e)	Tm IV
\mathbf{B}_{19}	$-(x_7 - \frac{1}{2})\mathbf{a}_1 + x_7\mathbf{a}_2 + x_7\mathbf{a}_3$	$=$	$ax_7\hat{x} + \frac{1}{4}a\hat{y} + \frac{1}{4}a\hat{z}$	(24g)	Tm V
\mathbf{B}_{20}	$x_7\mathbf{a}_1 - (x_7 - \frac{1}{2})\mathbf{a}_2 - (x_7 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2})\hat{x} + \frac{1}{4}a\hat{y} + \frac{1}{4}a\hat{z}$	(24g)	Tm V
\mathbf{B}_{21}	$x_7\mathbf{a}_1 - (x_7 - \frac{1}{2})\mathbf{a}_2 + x_7\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{x} + ax_7\hat{y} + \frac{1}{4}a\hat{z}$	(24g)	Tm V
\mathbf{B}_{22}	$-(x_7 - \frac{1}{2})\mathbf{a}_1 + x_7\mathbf{a}_2 - (x_7 - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{x} - a(x_7 - \frac{1}{2})\hat{y} + \frac{1}{4}a\hat{z}$	(24g)	Tm V
\mathbf{B}_{23}	$x_7\mathbf{a}_1 + x_7\mathbf{a}_2 - (x_7 - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{x} + \frac{1}{4}a\hat{y} + ax_7\hat{z}$	(24g)	Tm V
\mathbf{B}_{24}	$-(x_7 - \frac{1}{2})\mathbf{a}_1 - (x_7 - \frac{1}{2})\mathbf{a}_2 + x_7\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{x} + \frac{1}{4}a\hat{y} - a(x_7 - \frac{1}{2})\hat{z}$	(24g)	Tm V
\mathbf{B}_{25}	$z_8\mathbf{a}_1 + z_8\mathbf{a}_2 + (2x_8 - z_8)\mathbf{a}_3$	$=$	$ax_8\hat{x} + ax_8\hat{y} + az_8\hat{z}$	(48h)	Ni III
\mathbf{B}_{26}	$z_8\mathbf{a}_1 + z_8\mathbf{a}_2 - (2x_8 + z_8)\mathbf{a}_3$	$=$	$-ax_8\hat{x} - ax_8\hat{y} + az_8\hat{z}$	(48h)	Ni III

$$\begin{aligned}
\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

- [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.

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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.