

Th₂Ni₁₇ Structure:

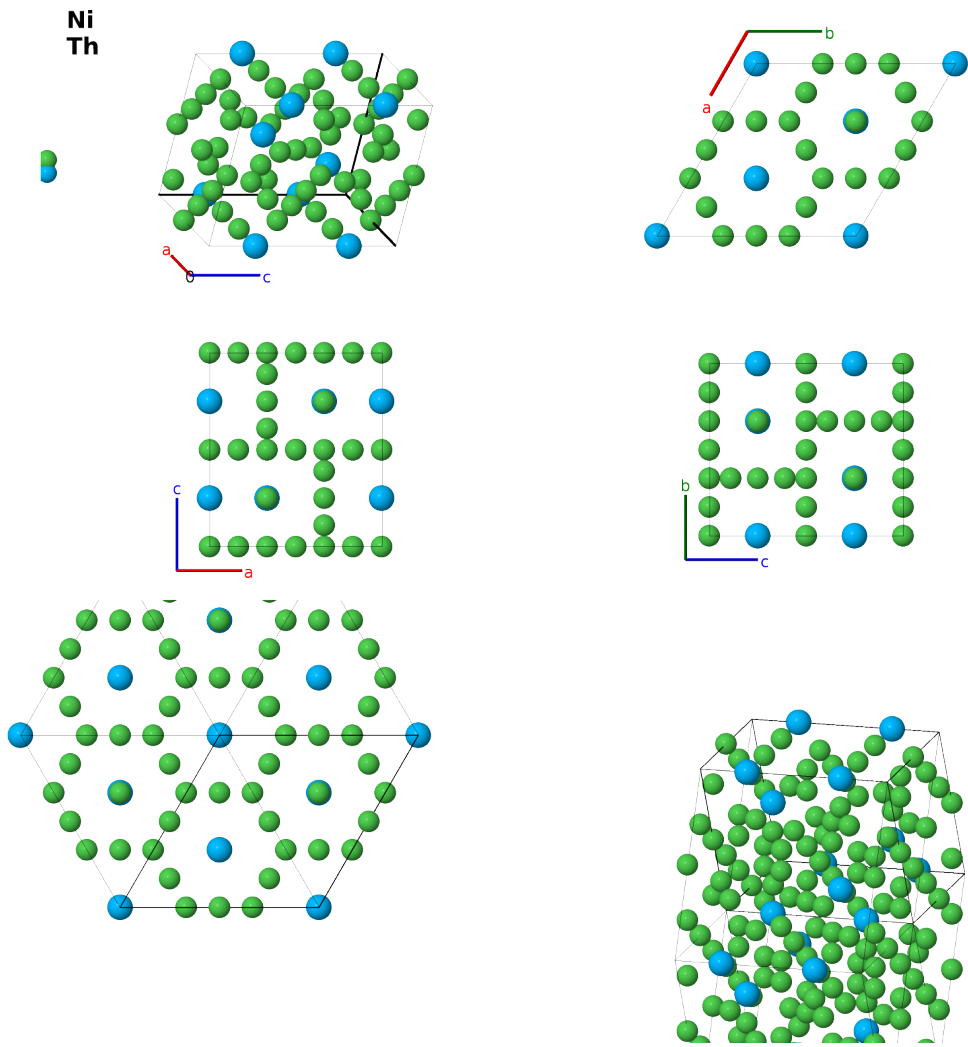
A17B2_hP38_194_fgjk_bc-001

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

https://aflow.org/prototype-encyclopedia/A17B2_hP38_194_fgjk_bc-001



Prototype	Ni ₁₇ Th ₂
AFLOW prototype label	A17B2_hP38_194_fgjk_bc-001
ICSD	105410
CCDC	1663299
Pearson symbol	hP38
Space group number	194

Space group symbol

$P6_3/mmc$

AFLOW prototype command

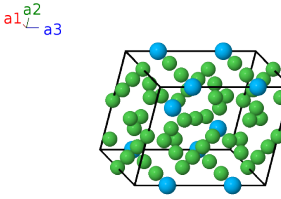
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--params= $a, c/a, z_3, x_5, y_5, x_6, z_6$

Other compounds with this structure

$\text{Ce}_2\text{Co}_{17}$, $\text{Ce}_2\text{Mg}_{17}$, $\text{Er}_2\text{Co}_{17}$, $\text{Gd}_2\text{Co}_{17}$, $\text{Gd}_2\text{Fe}_{17}$, $\text{Ho}_2\text{Co}_{17}$, $\beta\text{-Hf}_2\text{Be}_{17}$, $\text{La}_2\text{Fe}_{17}$, $\text{Lu}_2\text{Co}_{17}$, $\text{Nd}_2\text{Ni}_{17}$, $\text{Pr}_2\text{Co}_{17}$, $\text{Pu}_2\text{Co}_{17}$, $\text{Pu}_2\text{Ni}_{17}$, $\text{Sr}_2\text{Fe}_{17}$, $\text{Th}_2\text{Zn}_{17}$, $\beta\text{-Ti}_2\text{Be}_{17}$, $\text{Tm}_2\text{Co}_{17}$, U_2Zn_{17} , Y_2Co_{17} , Y_2Ni_{17}

- This is an idealized form of the $\text{Th}_2\text{Ni}_{17}$ structure. The actual composition can be as nickel rich as $\text{Th}_2\text{Ni}_{19}$. (Givord, 1972)
- This is a superstructure of CaCu_5 ($D2_d$) with nickel dimers aligned along the z -axis replacing thorium atoms. (Florio, 1956)

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(2b)	Th I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(2b)	Th I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	Th II
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	Th II
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4f)	Ni I
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Ni I
$\mathbf{B}_7$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4f)	Ni I
$\mathbf{B}_8$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Ni I
$\mathbf{B}_9$	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}}$	(6g)	Ni II
$\mathbf{B}_{10}$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}}$	(6g)	Ni II
$\mathbf{B}_{11}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}}$	(6g)	Ni II
$\mathbf{B}_{12}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6g)	Ni II
$\mathbf{B}_{13}$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6g)	Ni II
$\mathbf{B}_{14}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6g)	Ni II
$\mathbf{B}_{15}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(12j)	Ni III
$\mathbf{B}_{16}$	$= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(12j)	Ni III
$\mathbf{B}_{17}$	$= -(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(12j)	Ni III
$\mathbf{B}_{18}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(12j)	Ni III
$\mathbf{B}_{19}$	$= y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(12j)	Ni III

$$\begin{aligned}
\mathbf{B}_{20} &= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}} &(12j) &\text{Ni III} \\
\mathbf{B}_{21} &= y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}} &(12j) &\text{Ni III} \\
\mathbf{B}_{22} &= (x_5 - y_5) \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}} &(12j) &\text{Ni III} \\
\mathbf{B}_{23} &= -x_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= -\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}} &(12j) &\text{Ni III} \\
\mathbf{B}_{24} &= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= -\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}} &(12j) &\text{Ni III} \\
\mathbf{B}_{25} &= -(x_5 - y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}} &(12j) &\text{Ni III} \\
\mathbf{B}_{26} &= x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}} &(12j) &\text{Ni III} \\
\mathbf{B}_{27} &= x_6 \mathbf{a}_1 + 2x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= \frac{3}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} &(12k) &\text{Ni IV} \\
\mathbf{B}_{28} &= -2x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= -\frac{3}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} &(12k) &\text{Ni IV} \\
\mathbf{B}_{29} &= x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= -\sqrt{3}ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} &(12k) &\text{Ni IV} \\
\mathbf{B}_{30} &= -x_6 \mathbf{a}_1 - 2x_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 &= -\frac{3}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} &(12k) &\text{Ni IV} \\
\mathbf{B}_{31} &= 2x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 &= \frac{3}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} &(12k) &\text{Ni IV} \\
\mathbf{B}_{32} &= -x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 &= \sqrt{3}ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} &(12k) &\text{Ni IV} \\
\mathbf{B}_{33} &= 2x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= \frac{3}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(12k) &\text{Ni IV} \\
\mathbf{B}_{34} &= -x_6 \mathbf{a}_1 - 2x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -\frac{3}{2}ax_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(12k) &\text{Ni IV} \\
\mathbf{B}_{35} &= -x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= \sqrt{3}ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(12k) &\text{Ni IV} \\
\mathbf{B}_{36} &= -2x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3 &= -\frac{3}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}} &(12k) &\text{Ni IV} \\
\mathbf{B}_{37} &= x_6 \mathbf{a}_1 + 2x_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3 &= \frac{3}{2}ax_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}} &(12k) &\text{Ni IV} \\
\mathbf{B}_{38} &= x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3 &= -\sqrt{3}ax_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}} &(12k) &\text{Ni IV}
\end{aligned}$$

References

- [1] J. V. Florio, N. C. Baenziger, and R. E. Rundle, *Compounds of thorium with transition metals. II. Systems with iron, cobalt and nickel*, Acta Cryst. **9**, 367–372 (1972), doi:10.1107/S0365110X5600108X.

Found in

- [1] D. Givord, F. Givord, R. Lemaire, W. J. James, and J. S. Shah, *Evidence of disordered substitutions in the “Th₂Ni₁₇-type” structure. Exact structure determination of the Th-Ni, Y-Ni and Er-Co compounds*, J. Less-Common Met. **29**, 389–396 (1972), doi:10.1016/0022-5088(72)90202-0.

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