Th$_2$Ni$_{17}$ Structure: A17B2_hP38_194_fgjk_bc-001

https://aflow.org/p/DQFR

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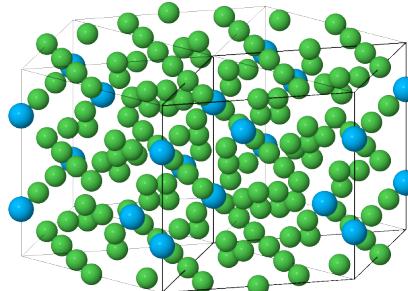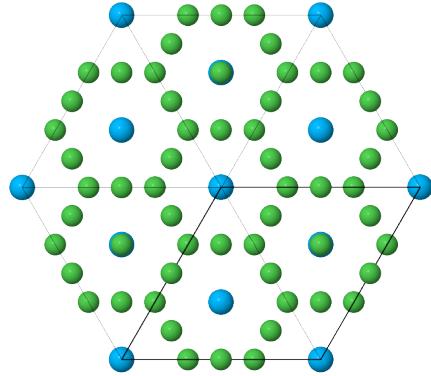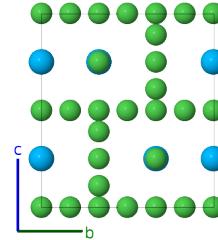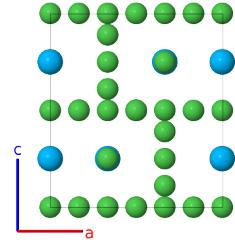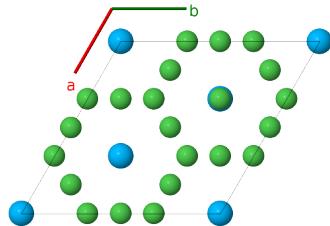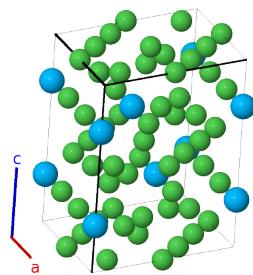
Prototype	Ni$_{17}$Th$_2$
AFLOW prototype label	A17B2_hP38_194_fgjk_bc-001
ICSD	105410
Pearson symbol	hP38
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	aflow --proto=A17B2_hP38_194_fgjk_bc-001 --params=$a, c/a, z_3, x_5, y_5, x_6, z_6$

Other compounds with this structure

Ce_2Co_{17}, Ce_2Mg_{17}, Er_2Co_{17}, Gd_2Co_{17}, Gd_2Fe_{17}, Ho_2Co_{17}, β-Hf_2Be_{17}, La_2Fe_{17}, Lu_2Co_{17}, Nd_2Ni_{17}, Pu_2Co_{17}, Pu_2Ni_{17}, Sr_2Fe_{17}, Th_2Zn_{17}, β-Ti_2Be_{17}, Tm_2Co_{17}, U_2Zn_{17}, Y_2Co_{17}, Y_2Ni_{17}

- This is an idealized form of the Th_2Ni_{17} structure. The actual composition can be as nickel rich as Th_2Ni_{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

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
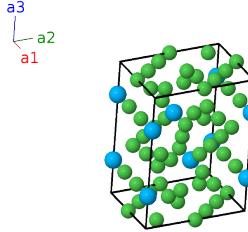
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$\tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{4}c\,\hat{\mathbf{z}}$	(2b)	Th I
$\mathbf{B_2}$	$=$	$\tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{3}{4}c\,\hat{\mathbf{z}}$	(2b)	Th I
$\mathbf{B_3}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Th II
$\mathbf{B_4}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Th II
$\mathbf{B_5}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4f)	Ni I
$\mathbf{B_6}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \left(z_3 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4f)	Ni I
$\mathbf{B_7}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4f)	Ni I
$\mathbf{B_8}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} - \left(z_3 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4f)	Ni I
$\mathbf{B_9}$	$=$	$\tfrac{1}{2}\mathbf{a_1}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(6g)	Ni II
$\mathbf{B_{10}}$	$=$	$\tfrac{1}{2}\mathbf{a_2}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(6g)	Ni II
$\mathbf{B_{11}}$	$=$	$\tfrac{1}{2}\mathbf{a_1} + \tfrac{1}{2}\mathbf{a_2}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}}$	(6g)	Ni II
$\mathbf{B_{12}}$	$=$	$\tfrac{1}{2}\mathbf{a_1} + \tfrac{1}{2}\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Ni II
$\mathbf{B_{13}}$	$=$	$\tfrac{1}{2}\mathbf{a_2} + \tfrac{1}{2}\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Ni II
$\mathbf{B_{14}}$	$=$	$\tfrac{1}{2}\mathbf{a_1} + \tfrac{1}{2}\mathbf{a_2} + \tfrac{1}{2}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Ni II
$\mathbf{B_{15}}$	$=$	$x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_5 + y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(12j)	Ni III
$\mathbf{B_{16}}$	$=$	$-y_5\,\mathbf{a_1} + \left(x_5 - y_5\right)\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_5 - 2y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(12j)	Ni III
$\mathbf{B_{17}}$	$=$	$-\left(x_5 - y_5\right)\mathbf{a_1} - x_5\,\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(2x_5 - y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(12j)	Ni III
$\mathbf{B_{18}}$	$=$	$-x_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_5 + y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(12j)	Ni III
$\mathbf{B_{19}}$	$=$	$y_5\,\mathbf{a_1} - \left(x_5 - y_5\right)\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(-x_5 + 2y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(12j)	Ni III
$\mathbf{B_{20}}$	$=$	$\left(x_5 - y_5\right)\mathbf{a_1} + x_5\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(2x_5 - y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(12j)	Ni III
$\mathbf{B_{21}}$	$=$	$y_5\,\mathbf{a_1} + x_5\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_5 + y_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(12j)	Ni III
$\mathbf{B_{22}}$	$=$	$\left(x_5 - y_5\right)\mathbf{a_1} - y_5\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_5 - 2y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(12j)	Ni III

$$\mathbf{B_{23}} = -x_5\,\mathbf{a_1} - (x_5 - y_5)\,\mathbf{a_2} + \tfrac{3}{4}\,\mathbf{a_3} = -\tfrac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}} \qquad \text{(12j)} \qquad \text{Ni III}$$

$$\mathbf{B_{24}} = -y_5\,\mathbf{a_1} - x_5\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3} = -\tfrac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}} \qquad \text{(12j)} \qquad \text{Ni III}$$

$$\mathbf{B_{25}} = -(x_5 - y_5)\,\mathbf{a_1} + y_5\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3} = \tfrac{1}{2}a\,(-x_5 + 2y_5)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}} \qquad \text{(12j)} \qquad \text{Ni III}$$

$$\mathbf{B_{26}} = x_5\,\mathbf{a_1} + (x_5 - y_5)\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3} = \tfrac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}} \qquad \text{(12j)} \qquad \text{Ni III}$$

$$\mathbf{B_{27}} = x_6\,\mathbf{a_1} + 2x_6\,\mathbf{a_2} + z_6\,\mathbf{a_3} = \tfrac{3}{2}ax_6\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \qquad \text{(12k)} \qquad \text{Ni IV}$$

$$\mathbf{B_{28}} = -2x_6\,\mathbf{a_1} - x_6\,\mathbf{a_2} + z_6\,\mathbf{a_3} = -\tfrac{3}{2}ax_6\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \qquad \text{(12k)} \qquad \text{Ni IV}$$

$$\mathbf{B_{29}} = x_6\,\mathbf{a_1} - x_6\,\mathbf{a_2} + z_6\,\mathbf{a_3} = -\sqrt{3}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \qquad \text{(12k)} \qquad \text{Ni IV}$$

$$\mathbf{B_{30}} = -x_6\,\mathbf{a_1} - 2x_6\,\mathbf{a_2} + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a_3} = -\tfrac{3}{2}ax_6\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad \text{(12k)} \qquad \text{Ni IV}$$

$$\mathbf{B_{31}} = 2x_6\,\mathbf{a_1} + x_6\,\mathbf{a_2} + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a_3} = \tfrac{3}{2}ax_6\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad \text{(12k)} \qquad \text{Ni IV}$$

$$\mathbf{B_{32}} = -x_6\,\mathbf{a_1} + x_6\,\mathbf{a_2} + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a_3} = \sqrt{3}ax_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad \text{(12k)} \qquad \text{Ni IV}$$

$$\mathbf{B_{33}} = 2x_6\,\mathbf{a_1} + x_6\,\mathbf{a_2} - z_6\,\mathbf{a_3} = \tfrac{3}{2}ax_6\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \qquad \text{(12k)} \qquad \text{Ni IV}$$

$$\mathbf{B_{34}} = -x_6\,\mathbf{a_1} - 2x_6\,\mathbf{a_2} - z_6\,\mathbf{a_3} = -\tfrac{3}{2}ax_6\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \qquad \text{(12k)} \qquad \text{Ni IV}$$

$$\mathbf{B_{35}} = -x_6\,\mathbf{a_1} + x_6\,\mathbf{a_2} - z_6\,\mathbf{a_3} = \sqrt{3}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \qquad \text{(12k)} \qquad \text{Ni IV}$$

$$\mathbf{B_{36}} = -2x_6\,\mathbf{a_1} - x_6\,\mathbf{a_2} - \left(z_6 - \tfrac{1}{2}\right)\mathbf{a_3} = -\tfrac{3}{2}ax_6\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad \text{(12k)} \qquad \text{Ni IV}$$

$$\mathbf{B_{37}} = x_6\,\mathbf{a_1} + 2x_6\,\mathbf{a_2} - \left(z_6 - \tfrac{1}{2}\right)\mathbf{a_3} = \tfrac{3}{2}ax_6\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad \text{(12k)} \qquad \text{Ni IV}$$

$$\mathbf{B_{38}} = x_6\,\mathbf{a_1} - x_6\,\mathbf{a_2} - \left(z_6 - \tfrac{1}{2}\right)\mathbf{a_3} = -\sqrt{3}ax_6\,\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad \text{(12k)} \qquad \text{Ni IV}$$

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 "Th$_2$Ni$_{17}$-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.