

Fe₃Th₇ (*D*10₂) Structure: A3B7_hP20_186_c_b2c-001

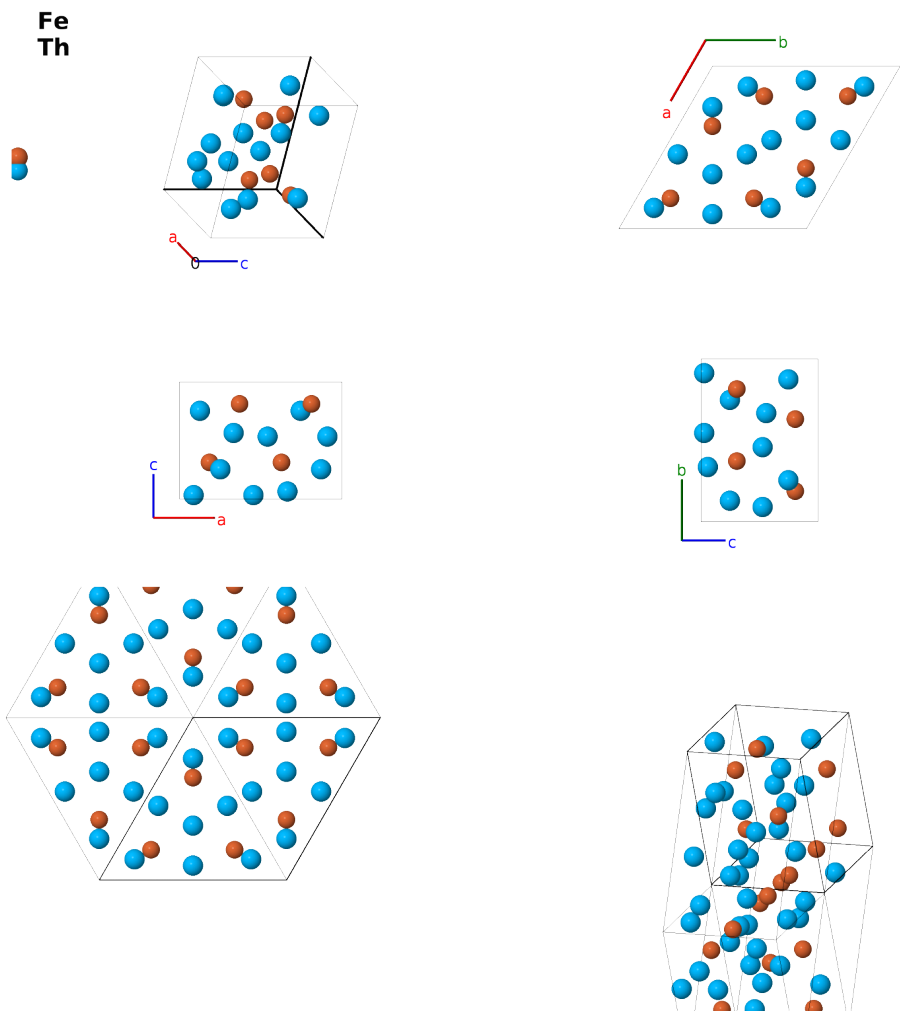
This structure previously used the label(s) A3B7_hP20_186_c_b2c. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A3B7_hP20_186_c_b2c-001



Prototype	Fe ₃ Th ₇
AFLOW prototype label	A3B7_hP20_186_c_b2c-001
Strukturbericht designation	<i>D</i> 10 ₂
ICSD	108477
CCDC	1666138

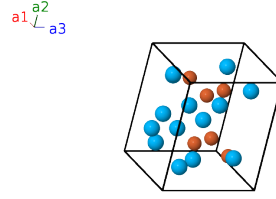
Pearson symbol	hP20
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	aflow --proto=A3B7_hP20_186_c_b2c-001 --params= $a, c/a, z_1, x_2, z_2, x_3, z_3, x_4, z_4$

Other compounds with this structure

B₃CoRh₆, B₃FeRh₆, B₃Ni₇, B₃Re₇, B₃Rh₇, B₃Ru₇, B₃Tc₇, C₃Fe₇, Co₃Nd₇, Co₃Th₇, Ir₃Ce₇, Ir₃La₇, Ir₃Pr₇, Ir₃Th₇, Ni₃Ce₇, Ni₃La₇, Ni₃Nd₇, Ni₃Pr₇, Ni₃Th₇, Os₃Th₇, Pd₃Ce₇, Pd₃Gd₇, Pd₃La₇, Pd₃Nd₇, Pd₃Pr₇, Pd₃Sm₇, Pd₃Tb₇, Pd₃Th₇, Pt₃La₇, Pt₃Nd₇, Pt₃Th₇, Rh₃Ce₇, Rh₃Dy₇, Rh₃Gd₇, Rh₃Ho₇, Rh₃La₇, Rh₃Nd₇, Rh₃Pr₇, Rh₃Sm₇, Rh₃Tb₇, Rh₃Th₇, Ru₃Th₇

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
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2b)	Th I
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Th I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-\sqrt{3}ax_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(6c)	Fe I
$\mathbf{B}_4$	$= x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(6c)	Fe I
$\mathbf{B}_5$	$= -2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(6c)	Fe I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\sqrt{3}ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Fe I
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 - 2x_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Fe I
$\mathbf{B}_8$	$= 2x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Fe I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-\sqrt{3}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6c)	Th II
$\mathbf{B}_{10}$	$= x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6c)	Th II
$\mathbf{B}_{11}$	$= -2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6c)	Th II
$\mathbf{B}_{12}$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\sqrt{3}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Th II
$\mathbf{B}_{13}$	$= -x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Th II
$\mathbf{B}_{14}$	$= 2x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Th II
$\mathbf{B}_{15}$	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-\sqrt{3}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6c)	Th III
$\mathbf{B}_{16}$	$= x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6c)	Th III
$\mathbf{B}_{17}$	$= -2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6c)	Th III
$\mathbf{B}_{18}$	$= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\sqrt{3}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Th III
$\mathbf{B}_{19}$	$= -x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Th III
$\mathbf{B}_{20}$	$= 2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Th III

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* **9**, 367–372 (1956), doi:10.1107/S0365110X5600108X.

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- [1] ICSD, *Inorganic Crystal Structure Database*. 108477.

First cited in

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