

ThB₄ (*D*1_{*e*}) Structure: A4B_tP20_127_ehj_g-001

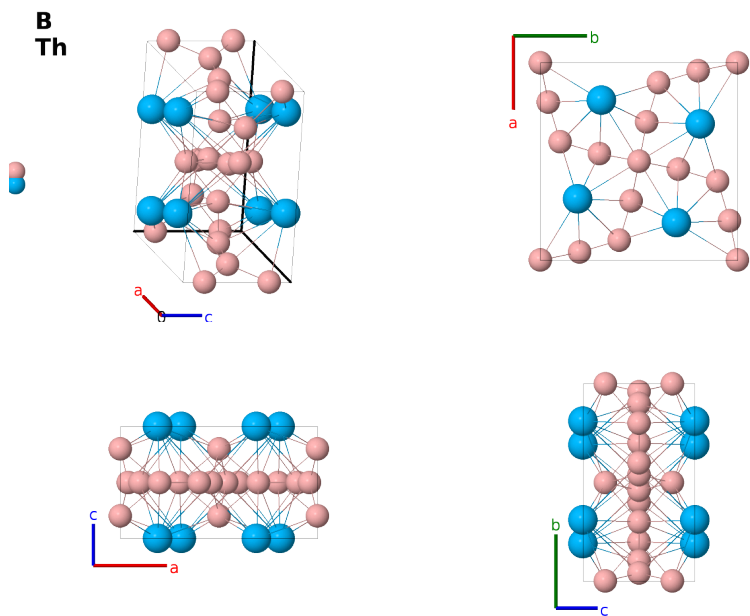
This structure previously used the label(s) **A4B_tP20_127_ehj_g**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A4B_tP20_127_ehj_g-001



Prototype	B ₄ Th
AFLOW prototype label	A4B_tP20_127_ehj_g-001
<i>Strukturbericht</i> designation	<i>D</i> 1 _{<i>e</i>}
ICSD	615570
CCDC	1746522
Pearson symbol	tP20
Space group number	127
Space group symbol	<i>P</i> 4/ <i>mbm</i>
AFLOW prototype command	<code>aflow --proto=A4B_tP20_127_ehj_g-001</code> <code>--params=<i>a</i>, <i>c/a</i>, <i>z</i>₁, <i>x</i>₂, <i>x</i>₃, <i>x</i>₄, <i>y</i>₄</code>

Other compounds with this structure

CeB₄, DyB₄, ErB₄, GdB₄, HoB₄, LaB₄, NdB₄, PrB₄, PuB₄, SmB₄, TbB₄, TmB₄, UB₄, YB₄, YbB₄

Simple Tetragonal primitive vectors



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(4e)	B I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(4e)	B I
$\mathbf{B}_3$	$= -z_1 \mathbf{a}_3$	$=$	$-c z_1 \hat{\mathbf{z}}$	(4e)	B I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(4e)	B I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2$	$=$	$a x_2 \hat{\mathbf{x}} + a (x_2 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Th I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2$	$=$	$-a x_2 \hat{\mathbf{x}} - a (x_2 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Th I
$\mathbf{B}_7$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$-a (x_2 - \frac{1}{2}) \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}}$	(4g)	Th I
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$a (x_2 + \frac{1}{2}) \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}}$	(4g)	Th I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + a (x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	B II
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - a (x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	B II
$\mathbf{B}_{11}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	B II
$\mathbf{B}_{12}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	B II
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + a y_4 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	B III
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - a y_4 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	B III
$\mathbf{B}_{15}$	$= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a y_4 \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	B III
$\mathbf{B}_{16}$	$= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a y_4 \hat{\mathbf{x}} - a x_4 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	B III
$\mathbf{B}_{17}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	B III
$\mathbf{B}_{18}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	B III
$\mathbf{B}_{19}$	$= (y_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (y_4 + \frac{1}{2}) \hat{\mathbf{x}} + a (x_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	B III
$\mathbf{B}_{20}$	$= -(y_4 - \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (y_4 - \frac{1}{2}) \hat{\mathbf{x}} - a (x_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8j)	B III

References

- [1] A. Zalkin and D. H. Templeton, *The Crystal Structures of CeB₄, ThB₄, and UB₄*, J. Chem. Phys. **18**, 391 (1950), doi:10.1063/1.1747637.

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