

Tetragonal Ba₃Zr₂S₇ Structure: A3B7C2_tP48_136_fj_2eghj-j-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/Z7PY>

https://aflow.org/prototype-encyclopedia/A3B7C2_tP48_136_fj_2eghj-j-001

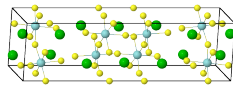
Prototype	Ba ₃ S ₇ Zr ₂
AFLOW prototype label	A3B7C2_tP48_136_fj_2eghj-j-001
ICSD	59271
CCDC	1623114
Pearson symbol	tP48
Space group number	136
Space group symbol	$P4_2/mnm$
AFLOW prototype command	<pre>aflow --proto=A3B7C2_tP48_136_fj_2eghj-j-001 --params=a, c/a, z₁, z₂, x₃, x₄, z₅, x₆, z₆, x₇, z₇, x₈, z₈</pre>

- The ICSD says the prototype of this structure is SrTb₂Fe₂O₇, but the structures are in fact quite different so we place this structure in its own prototype.
- This is the low temperature form of Ba₃Zr₂S₇, with data apparently taken at room temperature, though the ICSD entry says it was taken at 153K. At higher temperatures the structure becomes orthorhombic.

Simple Tetragonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$

a1
a2
a3



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	$z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(4e) S I

$\mathbf{B}_2 =$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c (z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B}_3 =$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - c (z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B}_4 =$	$-z_1 \mathbf{a}_3$	$=$	$-cz_1 \hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B}_5 =$	$z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B}_6 =$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B}_7 =$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - c (z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B}_8 =$	$-z_2 \mathbf{a}_3$	$=$	$-cz_2 \hat{\mathbf{z}}$	(4e)	S II
$\mathbf{B}_9 =$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}}$	(4f)	Ba I
$\mathbf{B}_{10} =$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}}$	(4f)	Ba I
$\mathbf{B}_{11} =$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Ba I
$\mathbf{B}_{12} =$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Ba I
$\mathbf{B}_{13} =$	$x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}}$	(4g)	S III
$\mathbf{B}_{14} =$	$-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}}$	(4g)	S III
$\mathbf{B}_{15} =$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} + a (x_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	S III
$\mathbf{B}_{16} =$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} - a (x_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	S III
$\mathbf{B}_{17} =$	$\frac{1}{2} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8h)	S IV
$\mathbf{B}_{18} =$	$\frac{1}{2} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8h)	S IV
$\mathbf{B}_{19} =$	$\frac{1}{2} \mathbf{a}_1 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - c (z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8h)	S IV
$\mathbf{B}_{20} =$	$\frac{1}{2} \mathbf{a}_1 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_5 \hat{\mathbf{z}}$	(8h)	S IV
$\mathbf{B}_{21} =$	$\frac{1}{2} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8h)	S IV
$\mathbf{B}_{22} =$	$\frac{1}{2} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} - c (z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8h)	S IV
$\mathbf{B}_{23} =$	$\frac{1}{2} \mathbf{a}_1 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8h)	S IV
$\mathbf{B}_{24} =$	$\frac{1}{2} \mathbf{a}_1 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + cz_5 \hat{\mathbf{z}}$	(8h)	S IV
$\mathbf{B}_{25} =$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8j)	Ba II
$\mathbf{B}_{26} =$	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8j)	Ba II
$\mathbf{B}_{27} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_6 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_6 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	Ba II
$\mathbf{B}_{28} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_6 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_6 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	Ba II
$\mathbf{B}_{29} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_6 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_6 + \frac{1}{2}) \hat{\mathbf{y}} - c (z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	Ba II
$\mathbf{B}_{30} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_6 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_6 - \frac{1}{2}) \hat{\mathbf{y}} - c (z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	Ba II
$\mathbf{B}_{31} =$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8j)	Ba II
$\mathbf{B}_{32} =$	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8j)	Ba II
$\mathbf{B}_{33} =$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8j)	S V
$\mathbf{B}_{34} =$	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8j)	S V
$\mathbf{B}_{35} =$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_7 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_7 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	S V
$\mathbf{B}_{36} =$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_7 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_7 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8j)	S V

$$\begin{aligned}
\mathbf{B}_{37} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_7 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_7 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8j) &\quad \text{S V} \\
\mathbf{B}_{38} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8j) &\quad \text{S V} \\
\mathbf{B}_{39} &= x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= ax_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(8j) &\quad \text{S V} \\
\mathbf{B}_{40} &= -x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -ax_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(8j) &\quad \text{S V} \\
\mathbf{B}_{41} &= x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} &(8j) &\quad \text{Zr I} \\
\mathbf{B}_{42} &= -x_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} &(8j) &\quad \text{Zr I} \\
\mathbf{B}_{43} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_8 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8j) &\quad \text{Zr I} \\
\mathbf{B}_{44} &= \left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_8 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8j) &\quad \text{Zr I} \\
\mathbf{B}_{45} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_8 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8j) &\quad \text{Zr I} \\
\mathbf{B}_{46} &= \left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_8 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8j) &\quad \text{Zr I} \\
\mathbf{B}_{47} &= x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} &(8j) &\quad \text{Zr I} \\
\mathbf{B}_{48} &= -x_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} &(8j) &\quad \text{Zr I}
\end{aligned}$$

References

- [1] Y.-C. Hung, J. C. Fetting, and B. W. Eichhorn, *Ba₃Zr₂S₇, the Low-Temperature Polymorph*, Acta Crystallogr. Sect. C **53**, 827–829 (1997), doi:10.1107/S0108270197003089.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).

Ba
S
Zr

