

Orthorhombic Ba₃Zr₂S₇ Structure:

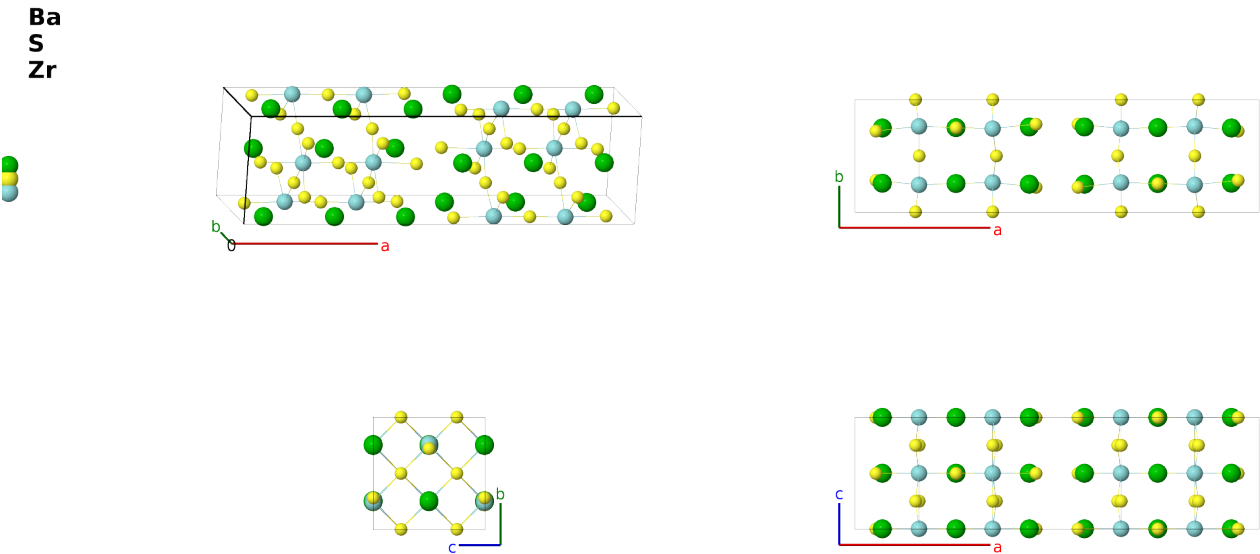
A3B7C2_oC48_66_el_f2gl_l-001

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<https://aflow.org/prototype-encyclopedia/2ZLH>

https://aflow.org/prototype-encyclopedia/A3B7C2_oC48_66_el_f2gl_l-001

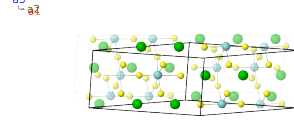


Prototype	Ba ₃ S ₇ Zr ₂
AFLOW prototype label	A3B7C2_oC48_66_el_f2gl_l-001
ICSD	69854
CCDC	1631691
Pearson symbol	oC48
Space group number	66
Space group symbol	<i>Cccm</i>
AFLOW prototype command	<pre>aflow --proto=A3B7C2_oC48_66_el_f2gl_l-001 --params=a, b/a, c/a, x₃, x₄, x₅, y₅, x₆, y₆, x₇, y₇</pre>

- The individual layers of this structure resemble cubic perovskite ($E2_1$), and orthorhombic Ba₃Zr₂S₇ is a Ruddlesden-Popper structure.
- At low temperatures this transforms to a tetragonal structure.
- AFLOW shifts rotates the reported structure by 90° about the z-axis, so that the long axis is now in the x-direction, and then shifts the origin by (a/2,0,0).

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}}$	(4e)	Ba I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4e)	Ba I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}}$	(4f)	S I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4f)	S I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	S II
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	S II
$\mathbf{B}_7$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	S II
$\mathbf{B}_8$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	S II
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	S III
$\mathbf{B}_{10}$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	S III
$\mathbf{B}_{11}$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	S III
$\mathbf{B}_{12}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	S III
$\mathbf{B}_{13}$	$= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}}$	(8l)	Ba II
$\mathbf{B}_{14}$	$= -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}}$	(8l)	Ba II
$\mathbf{B}_{15}$	$= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8l)	Ba II
$\mathbf{B}_{16}$	$= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8l)	Ba II
$\mathbf{B}_{17}$	$= (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}}$	(8l)	S IV
$\mathbf{B}_{18}$	$= -(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}}$	(8l)	S IV
$\mathbf{B}_{19}$	$= -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8l)	S IV
$\mathbf{B}_{20}$	$= (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8l)	S IV
$\mathbf{B}_{21}$	$= (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}}$	(8l)	Zr I
$\mathbf{B}_{22}$	$= -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}}$	(8l)	Zr I
$\mathbf{B}_{23}$	$= -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8l)	Zr I
$\mathbf{B}_{24}$	$= (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8l)	Zr I

References

- [1] M. Saeki, Y. Yajima, and M. Onoda, *Preparation and crystal structures of new barium zirconium sulfides, Ba_2ZrS_4 and $Ba_3Zr_2S_7$* , J. Solid State Chem. **92**, 286–294 (1991), doi:10.1016/0022-4596(91)90336-G.

Found in

- [1] A. Jain, S. P. Ong, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, G. D. Ceder, and K. A. Persson, *Commentary: The Materials Project: A materials genome approach to accelerating materials innovation*, APL Materials **1**, 011002 (2013), doi:10.1063/1.4812323.

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