

Ba₅Si₃ Structure:

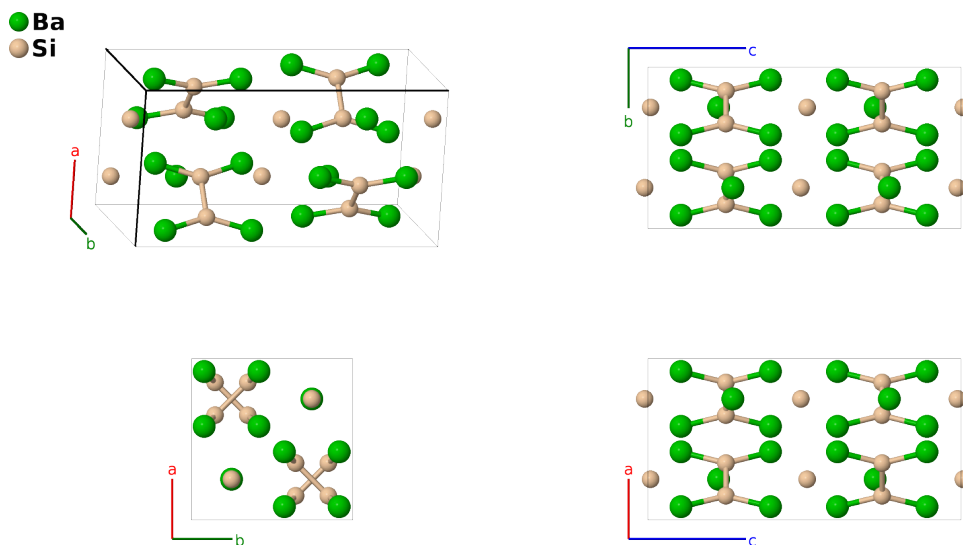
A5B3_tP32_130_cg_cf-001

This structure originally had the label A5B3_tP32_130_cg_cf. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

<https://aflow.org/p/0VYM>

https://aflow.org/p/A5B3_tP32_130_cg_cf-001

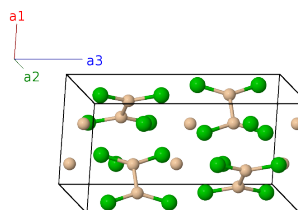


Prototype	Ba ₅ Si ₃
AFLOW prototype label	A5B3_tP32_130_cg_cf-001
ICSD	409377
Pearson symbol	tP32
Space group number	130
Space group symbol	<i>P4/ncc</i>
AFLOW prototype command	<code>aflow --proto=A5B3_tP32_130_cg_cf-001 --params=a, c/a, z₁, z₂, x₃, x₄, y₄, z₄</code>

- The ICSD entry seems to have displaced the *z*-coordinate of the Si II atom by 1/2.

Simple Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	Ba I
\mathbf{B}_2	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Ba I
\mathbf{B}_3	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	Ba I
\mathbf{B}_4	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Ba I
\mathbf{B}_5	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	Si I
\mathbf{B}_6	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Si I
\mathbf{B}_7	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	Si I
\mathbf{B}_8	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Si I
\mathbf{B}_9	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8f)	Si II
\mathbf{B}_{10}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8f)	Si II
\mathbf{B}_{11}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8f)	Si II
\mathbf{B}_{12}	$= -x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8f)	Si II
\mathbf{B}_{13}	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8f)	Si II
\mathbf{B}_{14}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8f)	Si II
\mathbf{B}_{15}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8f)	Si II
\mathbf{B}_{16}	$= x_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8f)	Si II
\mathbf{B}_{17}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16g)	Ba II
\mathbf{B}_{18}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16g)	Ba II
\mathbf{B}_{19}	$= -(y_4 - \frac{1}{2}) \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16g)	Ba II
\mathbf{B}_{20}	$= y_4 \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16g)	Ba II
\mathbf{B}_{21}	$= -x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	Ba II
\mathbf{B}_{22}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	Ba II
\mathbf{B}_{23}	$= (y_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	Ba II
\mathbf{B}_{24}	$= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	Ba II
\mathbf{B}_{25}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16g)	Ba II
\mathbf{B}_{26}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16g)	Ba II
\mathbf{B}_{27}	$= (y_4 + \frac{1}{2}) \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16g)	Ba II
\mathbf{B}_{28}	$= -y_4 \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16g)	Ba II
\mathbf{B}_{29}	$= x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	Ba II
\mathbf{B}_{30}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	Ba II
\mathbf{B}_{31}	$= -(y_4 - \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	Ba II
\mathbf{B}_{32}	$= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	Ba II

References

- [1] R. Nesper and F. Zürcher, *Refinement of the crystal structure of pentabarium trisilicide, Ba₅Si₃*, Z. Kristallogr. **214**, 20 (1966), doi:10.1515/ncrs-1999-0113.