Sr_5Si_3 Structure (*Obsolete*): A3B5_tI32_108_ac_a2c-001

This structure previously used the label(s) `A3B5_tI32_108_ac_a2c`. Calls to these addresses will be redirected here.

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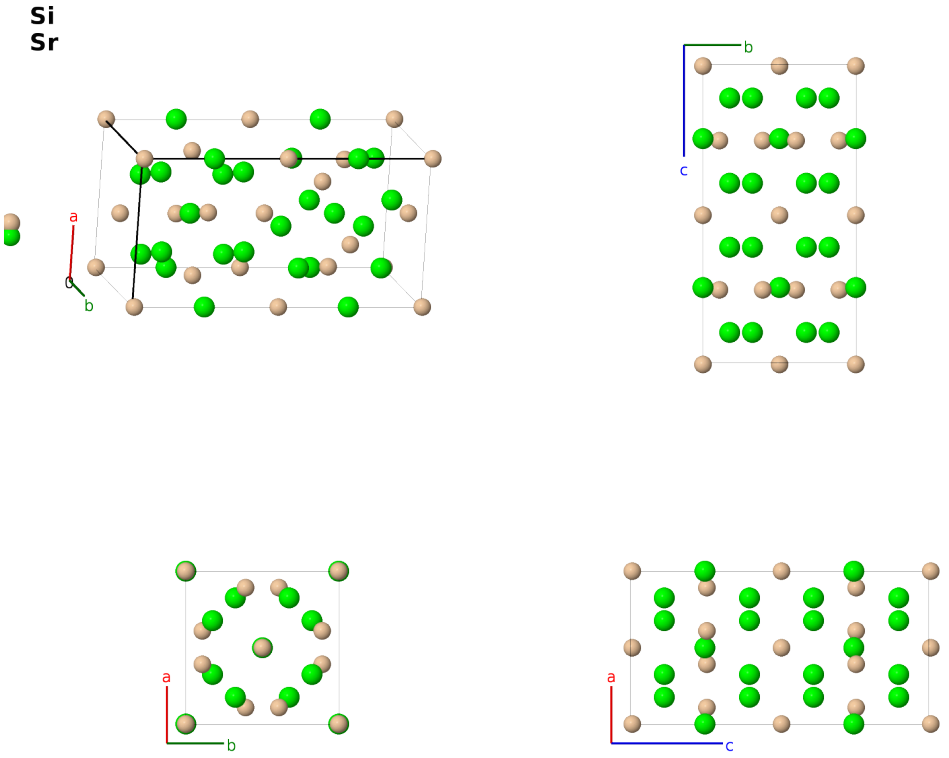
https://aflow.org/prototype-encyclopedia/BY2X

https://aflow.org/prototype-encyclopedia/A3B5_tI32_108_ac_a2c-001



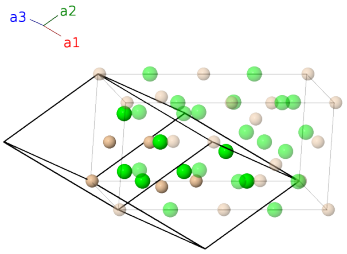
Prototype	Si_3Sr_5
AFLOW prototype label	A3B5_tI32_108_ac_a2c-001
ICSD	15639
CCDC	1596371
Pearson symbol	tI32
Space group number	108
Space group symbol	$I4cm$

AFLOW prototype command `aflow --proto=A3B5_tI32_108_ac_a2c-001 --params=`$a, c/a, z_1, z_2, x_3, z_3, x_4, z_4, x_5, z_5$

- This is the original determination of the Sr_5Si_3 (Nagorsen, 1967). Later(Nesper, 1999) re-examined the system and found that it is actually in the $D8_l$ Cr_5B_3 structure, space group $I4/mcm$ #140.
- We include this here as our first example of a structure in space group $I4cm$ #108.

Body-centered Tetragonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_1+\frac{1}{2}\right)\,\mathbf{a}_2$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$cz_2\,\hat{\mathbf{z}}$	(4a)	Sr I
$\mathbf{B_4}$	=	$\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_2$	=	$c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Sr I
$\mathbf{B_5}$	=	$\left(x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_1 +$ $(x_3+z_3)\,\mathbf{a}_2 + \left(2x_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8c)	Si II
$\mathbf{B_6}$	=	$\left(-x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_1 -$ $(x_3-z_3)\,\mathbf{a}_2 - \left(2x_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8c)	Si II
$\mathbf{B_7}$	=	$(x_3+z_3)\,\mathbf{a}_1 +$ $\left(-x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8c)	Si II
$\mathbf{B_8}$	=	$-(x_3-z_3)\,\mathbf{a}_1 +$ $\left(x_3+z_3+\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8c)	Si II
$\mathbf{B_9}$	=	$\left(x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1 +$ $(x_4+z_4)\,\mathbf{a}_2 + \left(2x_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Sr II
$\mathbf{B_{10}}$	=	$\left(-x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1 -$ $(x_4-z_4)\,\mathbf{a}_2 - \left(2x_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Sr II
$\mathbf{B_{11}}$	=	$(x_4+z_4)\,\mathbf{a}_1 +$ $\left(-x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Sr II
$\mathbf{B_{12}}$	=	$-(x_4-z_4)\,\mathbf{a}_1 +$ $\left(x_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	Sr II
$\mathbf{B_{13}}$	=	$\left(x_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_1 +$ $(x_5+z_5)\,\mathbf{a}_2 + \left(2x_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	Sr III
$\mathbf{B_{14}}$	=	$\left(-x_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_1 -$ $(x_5-z_5)\,\mathbf{a}_2 - \left(2x_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8c)	Sr III

$\mathbf{B_{15}}$	$= (x_5 + z_5)\,\mathbf{a}_1 + \left(-x_5 + z_5 + \frac{1}{2}\right)\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	$= -a\left(x_5 - \frac{1}{2}\right)\hat{\mathbf{x}} + a x_5\,\hat{\mathbf{y}} + c z_5\,\hat{\mathbf{z}}$	(8c)	Sr III
$\mathbf{B_{16}}$	$= -(x_5 - z_5)\,\mathbf{a}_1 + \left(x_5 + z_5 + \frac{1}{2}\right)\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	$= a\left(x_5 + \frac{1}{2}\right)\hat{\mathbf{x}} - a x_5\,\hat{\mathbf{y}} + c z_5\,\hat{\mathbf{z}}$	(8c)	Sr III

References

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Found in

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First cited in

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