V_4SiSb_2 Structure: A2BC4_tI28_140_h_a_k-001

This structure previously used the label(s) `A2BC4_tI28_140_h_a_k`. Calls to these addresses will be redirected here.

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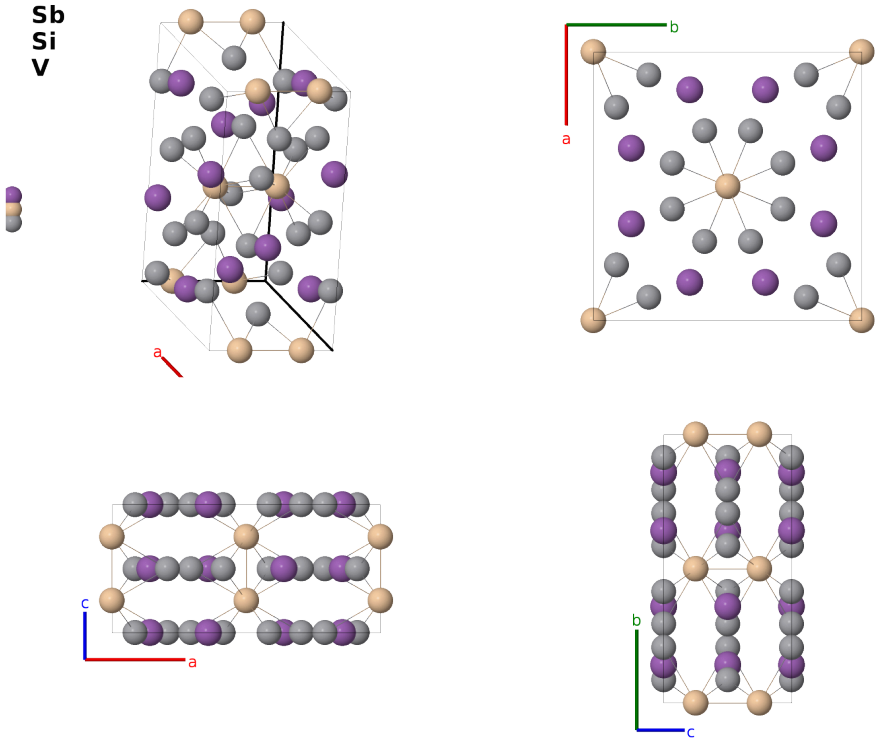
https://aflow.org/prototype-encyclopedia/VENL

https://aflow.org/prototype-encyclopedia/A2BC4_tI28_140_h_a_k-001



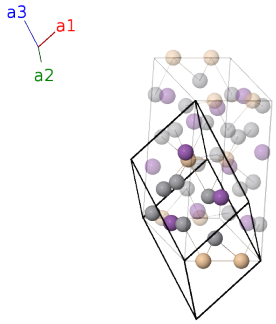
Prototype	Sb_2SiV_4
AFLOW prototype label	A2BC4_tI28_140_h_a_k-001
ICSD	82564
CCDC	1642648
Pearson symbol	tI28
Space group number	140
Space group symbol	$I4/mcm$
AFLOW prototype command	`aflow --proto=A2BC4_tI28_140_h_a_k-001 --params=`$a, c/a, x_2, x_3, y_3$

Other compounds with this structure
Nb_4SiSb_2, Ti_4CoBi_2, Ti_4CrBi_2, Ti_4FeBi_2, Ti_4MnBi_2, Ti_4NiBi_2

- This is the ternary version of the $D2_c$ U_6Mn structure. This can also be identified as a version of the $D8_m$ W_5Si_3 structure with defects.

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
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_3}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \left(2x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	Sb I
$\mathbf{B_4}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - \left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	Sb I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(8h)	Sb I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(8h)	Sb I
$\mathbf{B_7}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + (x_3 + y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}}$	(16k)	V I
$\mathbf{B_8}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - (x_3 + y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}}$	(16k)	V I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + (x_3 - y_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(16k)	V I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - (x_3 - y_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(16k)	V I
$\mathbf{B_{11}}$	=	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - (x_3 - y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(16k)	V I
$\mathbf{B_{12}}$	=	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_3 - y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(16k)	V I
$\mathbf{B_{13}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_3 + y_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(16k)	V I
$\mathbf{B_{14}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - (x_3 + y_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(16k)	V I

References

[1] P. Wollesen and W. Jeitschko, *V_4SiSb_2, a vanadium silicide antimonide crystallizing with a defect variant of the W_5Si_3-type structure*, J. Alloys Compd. **243**, 67–69 (1996), doi:10.1016/S0925-8388(96)02397-3.

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