

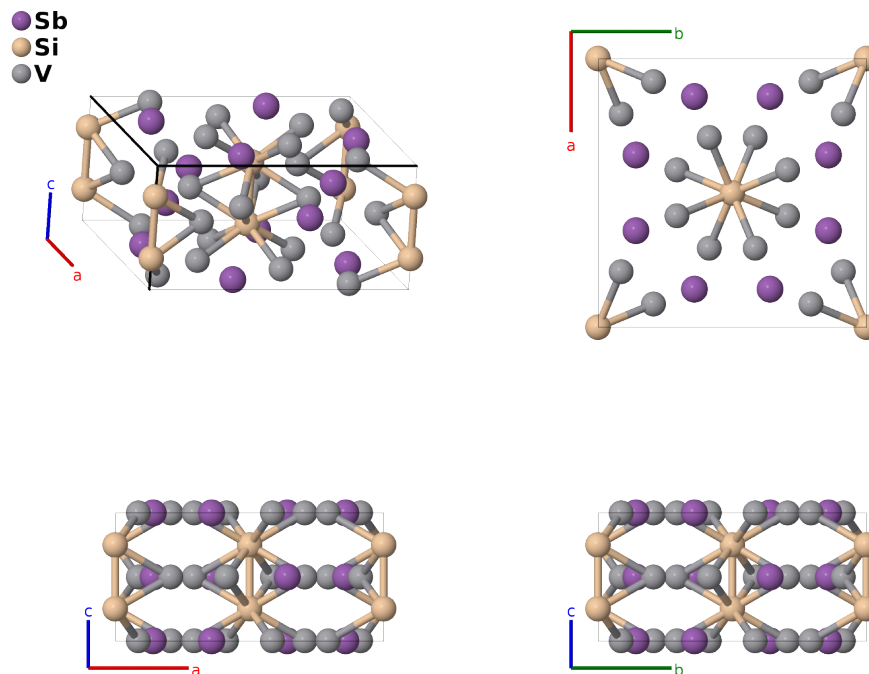
# V<sub>4</sub>SiSb<sub>2</sub> Structure: A2BC4\_tI28\_140\_h\_a\_k-001

This structure originally had the label **A2BC4\_tI28\_140\_h\_a\_k**. Calls to that address will be redirected here.

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<https://afLOW.org/p/VENL>

[https://afLOW.org/p/A2BC4\\_tI28\\_140\\_h\\_a\\_k-001](https://afLOW.org/p/A2BC4_tI28_140_h_a_k-001)



<b>Prototype</b>	Sb <sub>2</sub> SiV <sub>4</sub>
<b>AFLOW prototype label</b>	A2BC4_tI28_140_h_a_k-001
<b>ICSD</b>	82564
<b>Pearson symbol</b>	tI28
<b>Space group number</b>	140
<b>Space group symbol</b>	<i>I4/mcm</i>
<b>AFLOW prototype command</b>	<code>afLOW --proto=A2BC4_tI28_140_h_a_k-001 --params=a, c/a, x<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub></code>

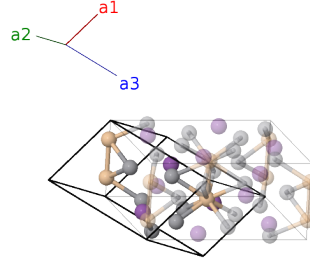
## Other compounds with this structure

Nb<sub>4</sub>SiSb<sub>2</sub>, Ti<sub>4</sub>CoBi<sub>2</sub>, Ti<sub>4</sub>CrBi<sub>2</sub>, Ti<sub>4</sub>FeBi<sub>2</sub>, Ti<sub>4</sub>MnBi<sub>2</sub>, Ti<sub>4</sub>NiBi<sub>2</sub>

- This is the ternary version of the  $D_{2c}$  U<sub>6</sub>Mn structure. This can also be identified as a version of the  $D_{8m}$  W<sub>5</sub>Si<sub>3</sub> structure with defects.

## Body-centered Tetragonal primitive vectors

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



## 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
$\mathbf{B}_3$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2 + (2x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	Sb I
$\mathbf{B}_4$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2 - (2x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	Sb I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(8h)	Sb I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}}$	(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
$\mathbf{B}_{11}$	$= (y_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(16k)	V I
$\mathbf{B}_{12}$	$= -(y_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(16k)	V I
$\mathbf{B}_{13}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(16k)	V I
$\mathbf{B}_{14}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - (x_3 + y_3) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(16k)	V I

## References

- [1] P. Wollesen and W. Jeitschko, *V<sub>4</sub>SiSb<sub>2</sub>, a vanadium silicide antimonide crystallizing with a defect variant of the W<sub>5</sub>Si<sub>3</sub>-type structure*, J. Alloys Compd. **243**, 67–69 (1996), doi:10.1016/S0925-8388(96)02397-3.