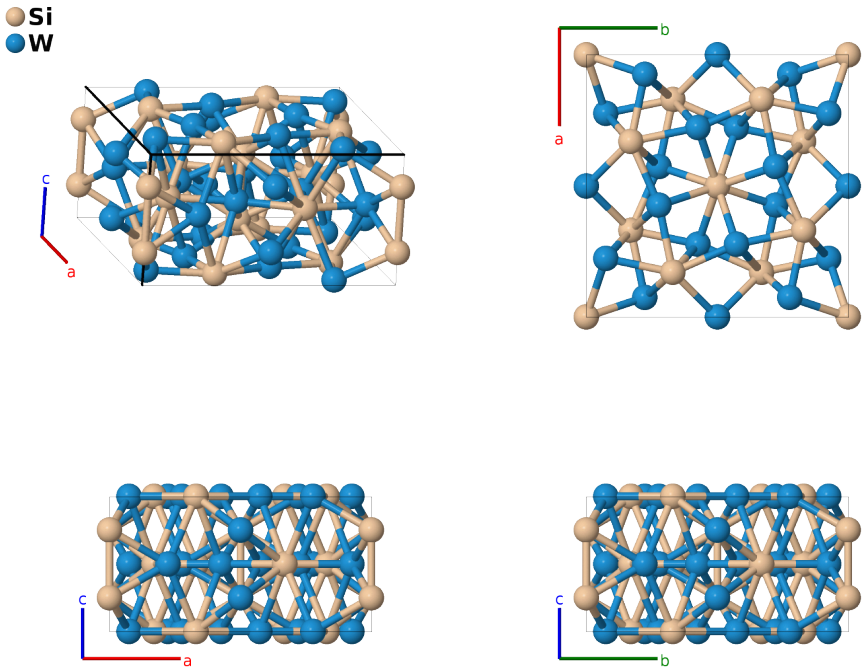
W_5Si_3 ($D8_m$) Structure: A3B5_tI32_140_ah_bk-001

This structure originally had the label `A3B5_tI32_140_ah_bk`. 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/4K4U

https://aflow.org/p/A3B5_tI32_140_ah_bk-001



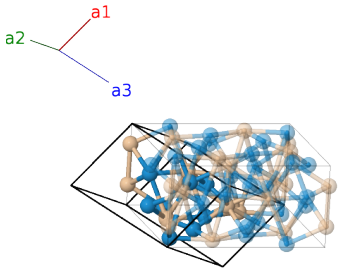
Prototype	Si_3W_5
AFLOW prototype label	A3B5_tI32_140_ah_bk-001
***Strukturbericht* designation**	$D8_m$
ICSD	73331
Pearson symbol	tI32
Space group number	140
Space group symbol	$I4/mcm$
AFLOW prototype command	`aflow --proto=A3B5_tI32_140_ah_bk-001 --params=`$a, c/a, x_3, x_4, y_4$

Other compounds with this structure

Cr_5Ge_3, Cr_5Si_3, Mo_5Si_3, Nb_5Si_3, Ta_5Si_3, Ti_5Ga_3, V_5Si_3, Ti_3Sb, $Hf_5Co_{1-x}Sb_{2+x}$, $Hf_5Cr_{1-x}Sb_{2+x}$, $Hf_5Cu_{1-x}Sb_{2+x}$, $Hf_5Fe_{1-x}Sb_{2+x}$, $Hf_5Ni_{1-x}Sb_{2+x}$, $Hf_5Pd_{1-x}Sb_{2+x}$, $Hf_5Rh_{1-x}Sb_{2+x}$, $Hf_5Ru_{1-x}Sb_{2+x}$, $Hf_5V_{1-x}Sb_{2+x}$, $Zr_5Co_{0.5}Sb_{2.5}$, $Zr_5Cr_{1-x}Bi_{2+x}$, $Zr_5Cr_{1-x}Sb_{2+x}$, $Zr_5Fe_{0.5}Sb_{2.5}$, $Zr_5Mn_{1-x}Bi_{2+x}$, $Zr_5Mn_{1-x}Sb_{2+x}$, $Zr_5Ni_{0.5}Sb_{2.5}$, $Zr_5Rh_{0.5}Sb_{2.5}$, $Zr_5Ru_{0.5}Sb_{2.5}$

- (Pearson, 1958) refers to this as the "T1 phase."
- Removing the atoms from the (4b) site transforms this into the $D2_c$ U_6Mn structure or the V_4SiSb_2 structure.

Body-centered Tetragonal primitive vectors



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

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
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	W I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	W I
$\mathbf{B_5}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(2x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	Si II
$\mathbf{B_6}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(2x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	Si II
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(8h)	Si II
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(8h)	Si II
$\mathbf{B_9}$	=	$y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + (x_4 + y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}}$	(16k)	W II
$\mathbf{B_{10}}$	=	$-y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - (x_4 + y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}}$	(16k)	W II
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + (x_4 - y_4)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(16k)	W II
$\mathbf{B_{12}}$	=	$-x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - (x_4 - y_4)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(16k)	W II
$\mathbf{B_{13}}$	=	$\left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - (x_4 - y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(16k)	W II
$\mathbf{B_{14}}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_4 - y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(16k)	W II
$\mathbf{B_{15}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_4 + y_4)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(16k)	W II
$\mathbf{B_{16}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - (x_4 + y_4)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(16k)	W II

References

[1] B. Aronsson, *The Crystal Structure of Mo_5Si_3 and W_5Si_3*, Acta Chem. Scand. **9**, 1107–1110 (1955), doi:10.3891/acta.chem.scand.09-1107.

Found in

[1] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, *International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 4 (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfort, 1958), 1964 reprint with corrections edn.