$TiSi_2$ ($C54$) Nowotony Chimney-Ladder Structure: A2B_oF24_70_e_a-001

This structure previously used the label(s) `A2B_oF24_70_e_a`. Calls to these addresses will be redirected here.

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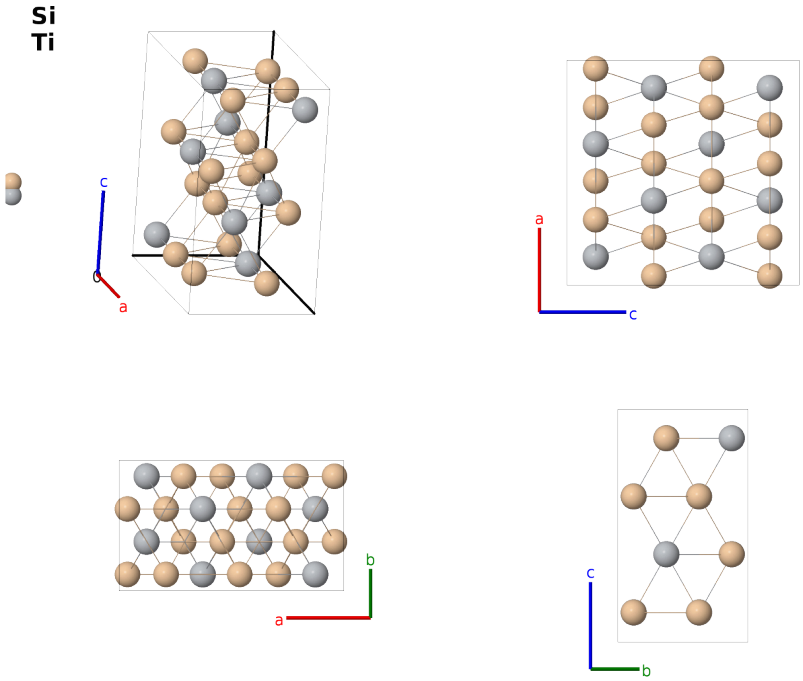
https://aflow.org/prototype-encyclopedia/KN7L

https://aflow.org/prototype-encyclopedia/A2B_oF24_70_e_a-001



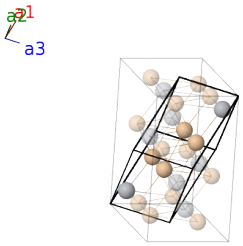
Prototype	Si_2Ti
AFLOW prototype label	A2B_oF24_70_e_a-001
***Strukturbericht* designation**	$C54$
ICSD	1089
CCDC	1591279
Pearson symbol	oF24
Space group number	70
Space group symbol	$Fddd$
AFLOW prototype command	`aflow --proto=A2B_oF24_70_e_a-001 --params=`$a, b/a, c/a, x_2$

Other compounds with this structure
$RuAl_2$, $RuGa_2$, $TiGe_2$, $ZrSn_2$

- This is the simplest example of a "Nowotny chimney-ladder structure" (Pearson, 1970), T_nX_m, where "T" is a transition metal, "X" is a row III or IV metal (or semiconductor), and $1.25 \leq m/n < 2$. The transition metal atoms are arranged similarly to the atoms in the β-Sn ($A5$).

Face-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(8a)	Ti I
$\mathbf{B_2}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$\frac{7}{8}a\,\hat{\mathbf{x}} + \frac{7}{8}b\,\hat{\mathbf{y}} + \frac{7}{8}c\,\hat{\mathbf{z}}$	(8a)	Ti I
$\mathbf{B_3}$	=	$-\left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Si I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Si I
$\mathbf{B_5}$	=	$\left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Si I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Si I

References

[1] W. Jeitschko, *Refinement of the crystal structure of $TiSi_2$ and some comments on bonding in $TiSi_2$ and related compounds*, Acta Crystallogr. Sect. B **33**, 2347–2348 (1977), doi:10.1107/S0567740877008462.

[2] W. B. Pearson, *Phases with Nowotny chimney-ladder structures considered as 'electron' phases*, Acta Crystallogr. Sect. B **26**, 1044–1046 (1970), doi:10.1107/S0567740870003564.

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