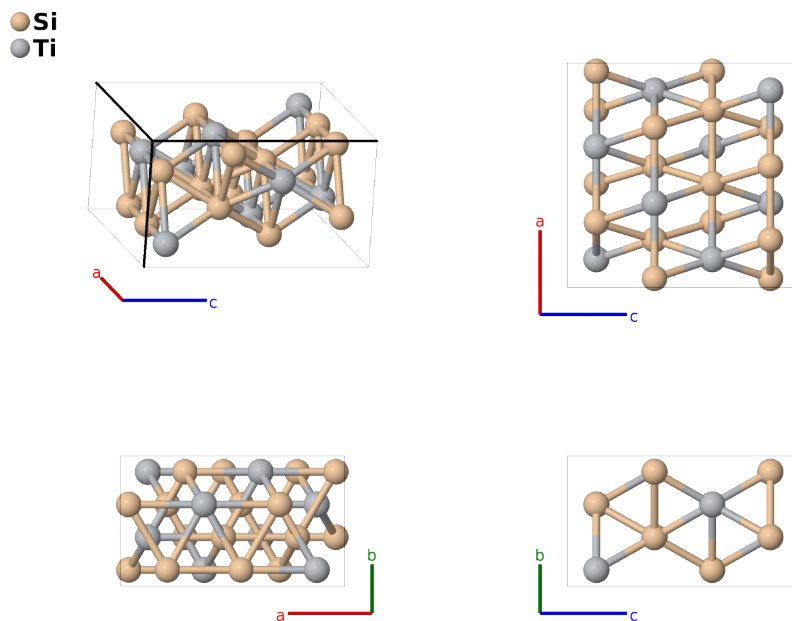# TiSi$_2$ ($C54$) Nowotony Chimney-Ladder Structure: A2B_oF24_70_e_a-001

This structure originally had the label `A2B_oF24_70_e_a`. Calls to that address will be redirected here.

https://aflow.org/p/KN7L

https://aflow.org/p/A2B_oF24_70_e_a-001

Prototype	Si$_2$Ti
AFLOW prototype label	A2B_oF24_70_e_a-001
***Strukturbericht* designation**	$C54$
ICSD	1089
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$_n$X$_m$, 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 ($A5$).
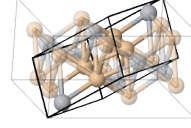
Face-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$

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

$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

Basis vectors

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