Hexagonal Ti_6Sn_5 Structure: A5B6_hP22_194_ach_gh-001

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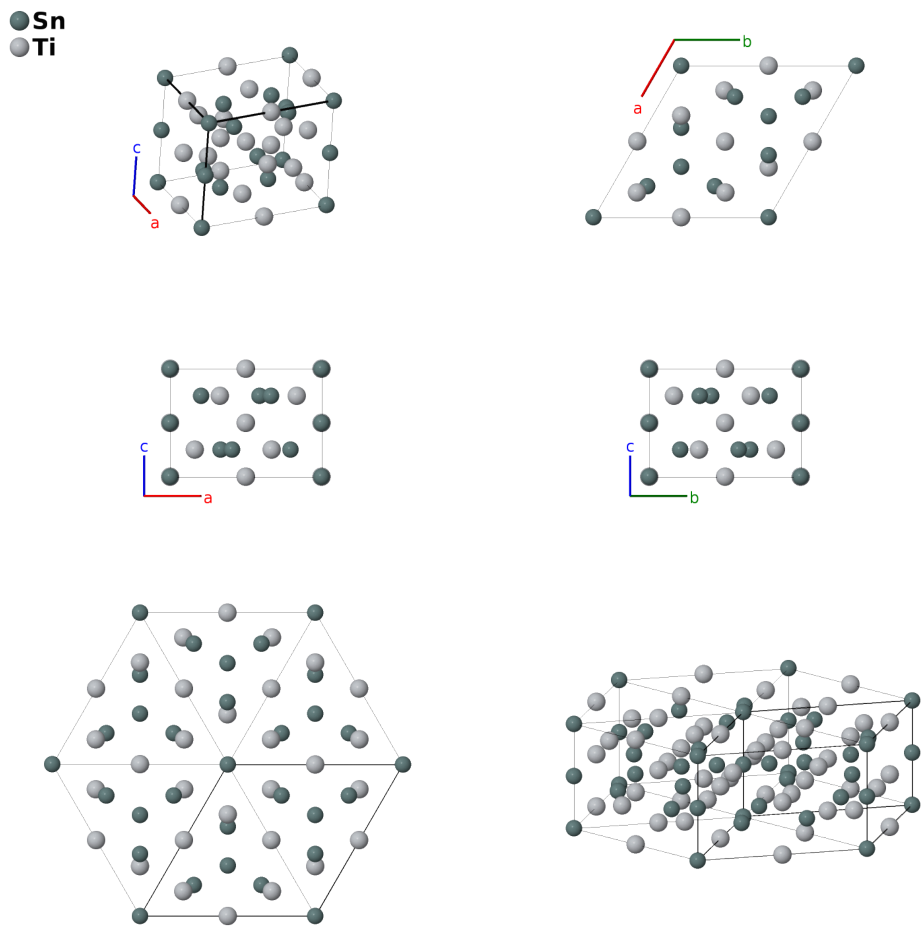
https://aflow.org/p/09JW

https://aflow.org/p/A5B6_hP22_194_ach_gh-001



Prototype	Sn_5Ti_6
AFLOW prototype label	A5B6_hP22_194_ach_gh-001
ICSD	660295
Pearson symbol	hP22
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=A5B6_hP22_194_ach_gh-001` `--params=`$a, c/a, x_4, x_5$

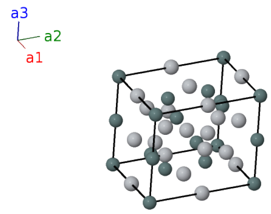
Other compounds with this structure

V_6Ga_5

- Hexagonal Ti_6Sn_5 coexists with orthorhombic Ti_6Sn_5, which takes on the Nb_6Sn_5 structure. (Oni, 2014)
- (van Vucht, 1964) state that the Sn-I atom is on the (4b) Wyckoff position, but the coordinates given are for the (2a) position. This fits with their figure of the structure, although the atoms they label at height "1/4" should be at zero and *vice versa*.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Sn I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Sn I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Sn II
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Sn II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(6g)	Ti I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(6g)	Ti I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(6g)	Ti I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Ti I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Ti I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Ti I
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1 + 2x_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn III
$\mathbf{B_{12}}$	=	$-2x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn III
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn III
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 - 2x_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn III
$\mathbf{B_{15}}$	=	$2x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn III
$\mathbf{B_{16}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\sqrt{3}ax_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Sn III
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + 2x_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Ti II
$\mathbf{B_{18}}$	=	$-2x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Ti II
$\mathbf{B_{19}}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Ti II
$\mathbf{B_{20}}$	=	$-x_5\,\mathbf{a}_1 - 2x_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Ti II
$\mathbf{B_{21}}$	=	$2x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Ti II
$\mathbf{B_{22}}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\sqrt{3}ax_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Ti II

References

[1] J. H. N. van Vucht, H. A. C. M. Bruning, H. C. Donkersloot, and A. H. G. de Mesquita, *The System Vanadium-Gallium*, Phillips Res. Repts. **19**, 407–421 (1964).

[2] A. A. Oni, D. Hook, J. P. Maria, and J. M. LeBeau, *Phase coexistence in* Ti_6Sn_5 *intermetallics*, Intermetallics **51**, 48–52 (2014), doi:10.1016/j.intermet.2014.03.002.