β-Sn ($A5$) Structure: A_tI4_141_a-001

This structure originally had the label `A_tI4_141_a`. Calls to that address will be redirected here.

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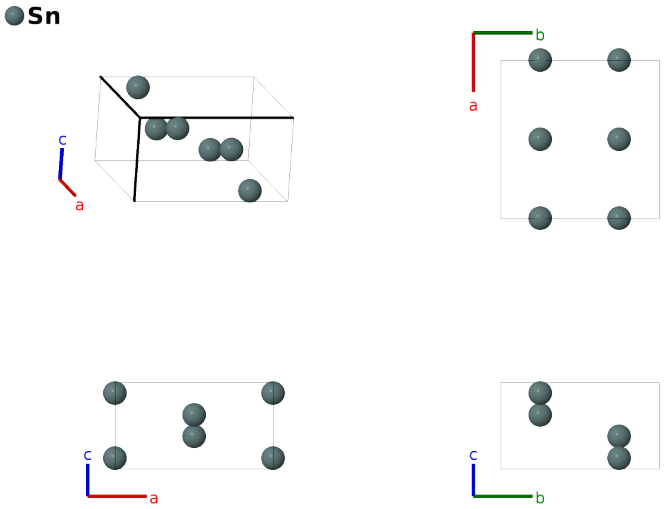
https://aflow.org/p/2BUF

https://aflow.org/p/A_tI4_141_a-001

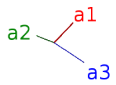


Prototype	Sn
AFLOW prototype label	A_tI4_141_a-001
***Strukturbericht* designation**	$A5$
ICSD	52486
Pearson symbol	tI4
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	`aflow --proto=A_tI4_141_a-001 --params=`$a, c/a$

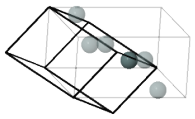
Other compounds with this structure
β-Ge

- When $c/a = \sqrt{2}$ this structure is equivalent to diamond ($A4$).
- The binary version of this structure is the GaSb (II) 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
$\mathbf{B_1}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(4a)	Sn I
$\mathbf{B_2}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(4a)	Sn I

References

[1] V. T. Deshpande and D. B. Sirdeshmukh, *Thermal Expansion of Tetragonal Tin*, Acta Cryst. **14**, 355–356 (1961), doi:10.1107/S0365110X61001212.

Found in

[1] M. Winter, *Tin: crystal structures* (1993-2022). WebElements: the periodic table on the WWW, The University of Sheffield and WebElements Ltd, UK.