

Simple Hexagonal (HgSn_{6-10} A_f) Structure: A_hP1_191_a-001

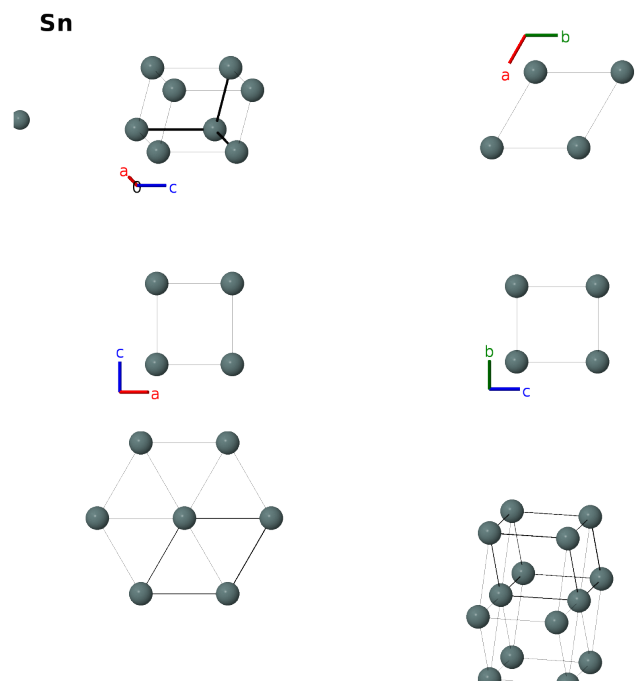
This structure previously used the label(s) **A_hP1_191_a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/3V7H>

https://aflow.org/prototype-encyclopedia/A_hP1_191_a-001



Prototype	HgSn_{6-10}
AFLOW prototype label	A_hP1_191_a-001
<i>Strukturbericht</i> designation	A_f
ICSD	639211
CCDC	1758642
Pearson symbol	hP1
Space group number	191
Space group symbol	$P6/mmm$
AFLOW prototype command	<code>aflow --proto=A_hP1_191_a-001 --params=a, c/a</code>

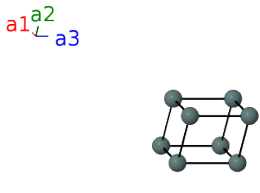
Other compounds with this structure

Si (metastable), disordered phases of BiIn, CdSn₁₉, In₇Sb₃, InSb

- Unlike the simple cubic lattice, there are no elements which take this structure as the ground state. There is a metastable silicon phase with this structure. The prototype state is a mercury-tin alloy. Thus the atom type “M” represents an average of Hg and Sn atoms.
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Hexagonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(1a) Sn I

References

- [1] G. V. Raynor and J. A. Lee, *The tin-rich intermediate phases in the alloys of tin with cadmium, indium and mercury*, Acta Metall. **2**, 616–620 (1954), doi:10.1016/0001-6160(54)90197-2.

Found in

- [1] P. Villars and L. Calvert, *Pearson’s Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017