

CoSn (*B35*) Structure: AB_hP6_191_f_ad-001

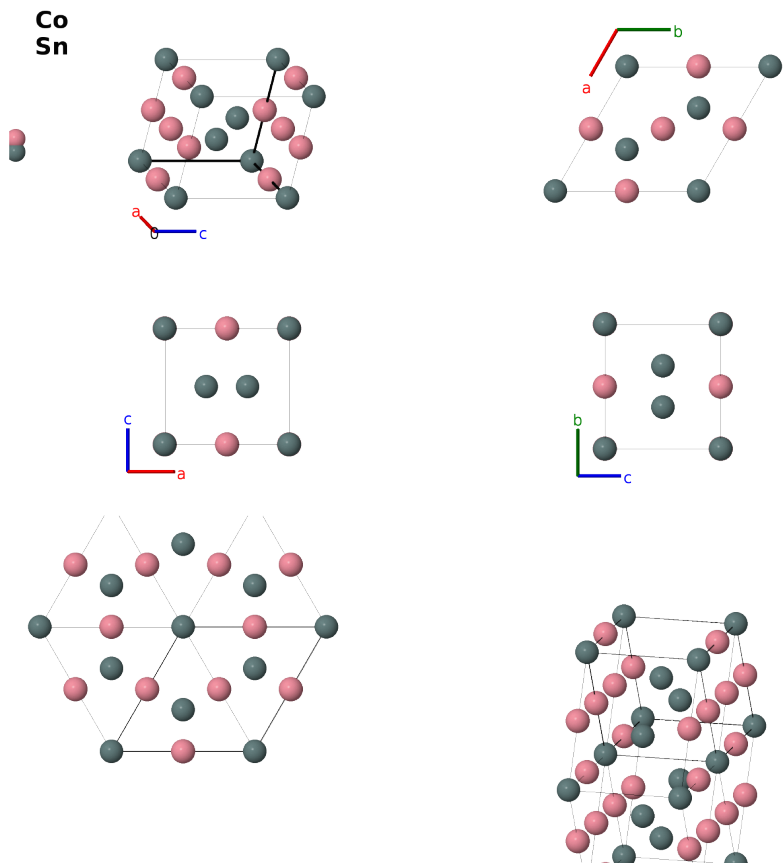
This structure previously used the label(s) **AB_hP6_191_f_ad**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/Z7YH>

https://aflow.org/prototype-encyclopedia/AB_hP6_191_f_ad-001



Prototype	CoSn
AFLOW prototype label	AB_hP6_191_f_ad-001
<i>Strukturbericht</i> designation	<i>B35</i>
ICSD	55564
CCDC	1619877
Pearson symbol	hP6
Space group number	191
Space group symbol	<i>P6/mmm</i>

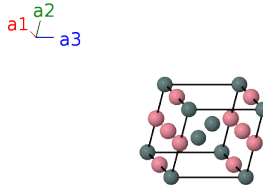
AFLOW prototype command `afLOW --proto=AB_hP6_191_f_ad-001`
 `--params= $a, c/a$`

Other compounds with this structure

CoGe, FeGe, FeSn, PbRh, NTa, PtTl, InNi

- The ternary form of this structure is Ti_2TaN_3 .

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
$\mathbf{B}_2$	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2d) Sn II
$\mathbf{B}_3$	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2d) Sn II
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}}$	(3f) Co I
$\mathbf{B}_5$	$=$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}}$	(3f) Co I
$\mathbf{B}_6$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}}$	(3f) Co I

References

- [1] A. Larsson, M. Haeberlein, S. Lidin, and U. Schwarz, *Single crystal structure refinement and high-pressure properties of CoSn*, J. Alloys Compd. **240**, 79–84 (1996), doi:10.1016/0925-8388(95)02189-2.

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