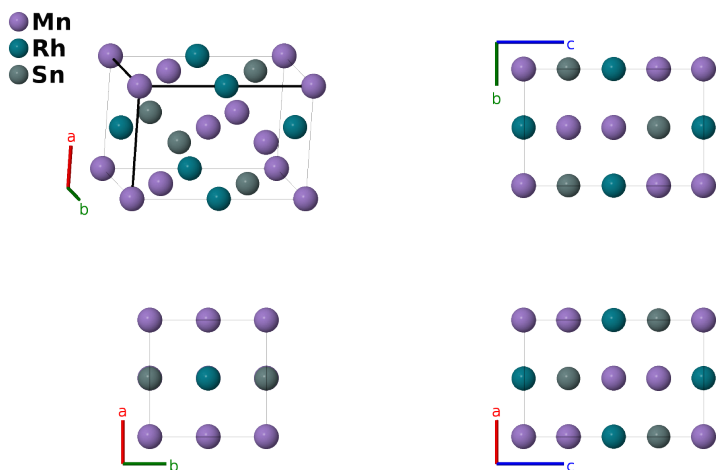


# Mn<sub>2</sub>RhSn Tetragonal Heusler Structure: A2BC\_tI8\_119\_ac\_b\_d-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://afLOW.org/p/4BRY>

[https://afLOW.org/p/A2BC\\_tI8\\_119\\_ac\\_b\\_d-001](https://afLOW.org/p/A2BC_tI8_119_ac_b_d-001)



<b>Prototype</b>	Mn <sub>2</sub> RhSn
<b>AFLOW prototype label</b>	A2BC_tI8_119_ac_b_d-001
<b>ICSD</b>	none
<b>Pearson symbol</b>	tI8
<b>Space group number</b>	119
<b>Space group symbol</b>	$\bar{I}4m2$
<b>AFLOW prototype command</b>	<code>afLOW --proto=A2BC_tI8_119_ac_b_d-001 --params=a, c/a</code>

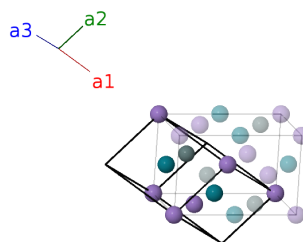
## Other compounds with this structure

Mn<sub>2</sub>PtIn, Mn<sub>3</sub>Ga, Rh<sub>2</sub>CrSn, Rh<sub>2</sub>FeSn, Mn<sub>2-x</sub>Rh<sub>1+x</sub>Sn, Mn<sub>2</sub>Rh<sub>x</sub>Co<sub>1-x</sub>Sn

- (Alijani, 2013) describe this as a tetragonal inverse Heusler compound. This is likely an idealized version of the structure, as the atoms are all assumed to sit on high-symmetry Wyckoff positions.

## Body-centered Tetragonal primitive vectors

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



---

**Basis vectors**

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) Mn I
$\mathbf{B}_2$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	=	$\frac{1}{2}c\hat{\mathbf{z}}$	(2b) Rh I
$\mathbf{B}_3$	=	$\frac{3}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(2c) Mn II
$\mathbf{B}_4$	=	$\frac{1}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}c\hat{\mathbf{z}}$	(2d) Sn I

**References**

- [1] V. Alijani, O. Meshcheriakova, J. Winterlik, G. Kreiner, G. H. Fecher, and C. Felser, *Increasing Curie temperature in tetragonal  $Mn_2RhSn$  Heusler compound through substitution of Rh by Co and Mn by Rh*, J. Appl. Phys. **113**, 063904 (2013), doi:10.1063/1.4791564.