Mn_2RhSn Tetragonal Heusler Structure: A2BC_tI8_119_ac_b_d-001

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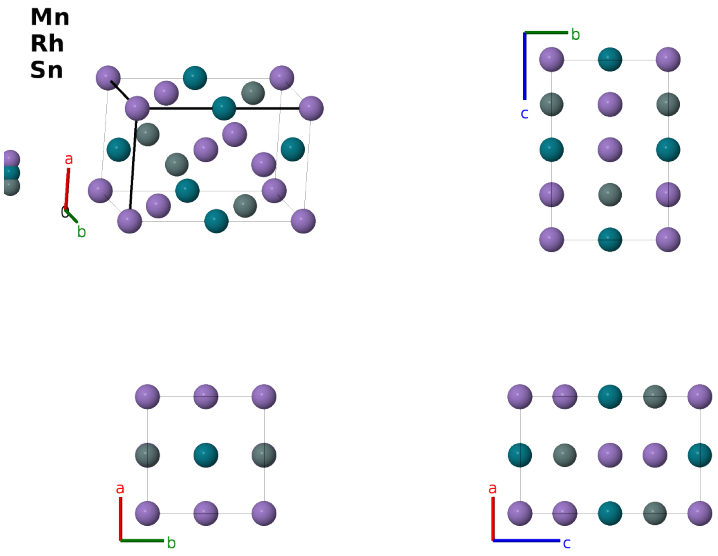
https://aflow.org/prototype-encyclopedia/4BRY

https://aflow.org/prototype-encyclopedia/A2BC_tI8_119_ac_b_d-001



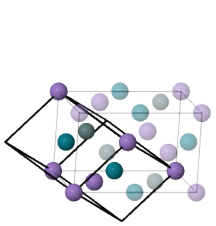
Prototype	Mn_2RhSn
AFLOW prototype label	A2BC_tI8_119_ac_b_d-001
Pearson symbol	tI8
Space group number	119
Space group symbol	$I\bar{4}m2$
AFLOW prototype command	`aflow --proto=A2BC_tI8_119_ac_b_d-001 --params=`$a, c/a$

Other compounds with this structure
Mn_2PtIn, Mn_3Ga, Rh_2CrSn, Rh_2FeSn, $Mn_{2-x}Rh_{1+x}Sn$, $Mn_2Rh_xCo_{1-x}Sn$

- (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

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	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.

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