$Mn_{1.4}PtSn$ Structure: A3B2C2_tI28_122_ad_c_d-001

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https://aflow.org/p/1YSS

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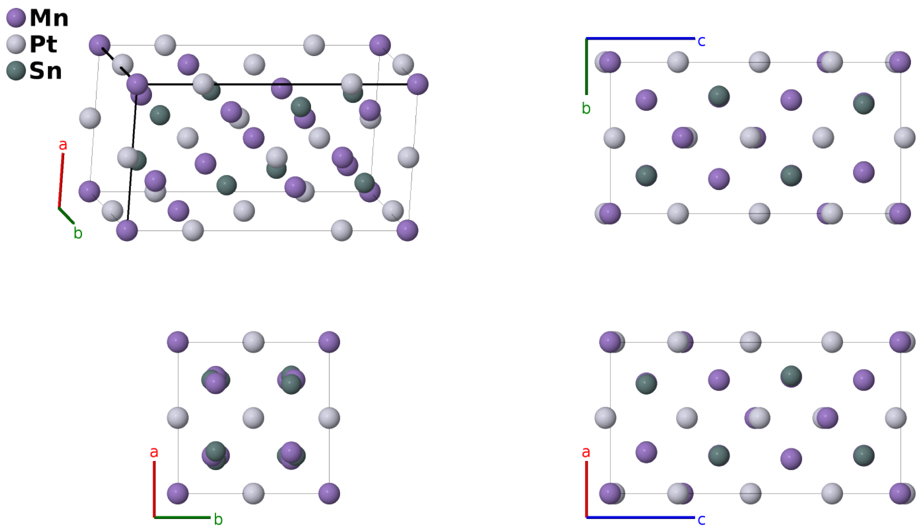
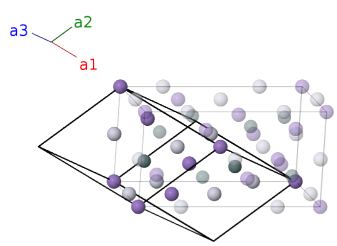


Prototype	$Mn_{1.4}PtSn$
AFLOW prototype label	A3B2C2_tI28_122_ad_c_d-001
ICSD	11061
Pearson symbol	tI28
Space group number	122
Space group symbol	$I\bar{4}2d$
AFLOW prototype command	`aflow --proto=A3B2C2_tI28_122_ad_c_d-001` `--params=`$a, c/a, z_2, x_3, x_4$

- (Vir, 2019) found that the Mn (4a) site (in the layer with the platinum (8c) atoms) has 20% vacancies, giving the noted departure from the nominal $Mn_3Pt_2Sn_2$ stoichiometry.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Mn I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{y}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(4a)	Mn I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$cz_2\,\mathbf{\hat{z}}$	(8c)	Pt I
$\mathbf{B_4}$	=	$-z_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_2$	=	$-cz_2\,\mathbf{\hat{z}}$	(8c)	Pt I
$\mathbf{B_5}$	=	$-\left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_1 - \left(z_2 - \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{y}} - c\left(z_2 - \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(8c)	Pt I
$\mathbf{B_6}$	=	$\left(z_2 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{y}} + c\left(z_2 + \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(8c)	Pt I
$\mathbf{B_7}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \left(x_3 + \frac{1}{8}\right)\,\mathbf{a}_2 + \left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_3\,\mathbf{\hat{x}} + \frac{1}{4}a\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(8d)	Mn II
$\mathbf{B_8}$	=	$\frac{7}{8}\,\mathbf{a}_1 - \left(x_3 - \frac{1}{8}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}} + \frac{3}{4}a\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(8d)	Mn II
$\mathbf{B_9}$	=	$-\left(x_3 - \frac{7}{8}\right)\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\mathbf{\hat{x}} - a\left(x_3 - \frac{1}{2}\right)\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(8d)	Mn II
$\mathbf{B_{10}}$	=	$\left(x_3 + \frac{7}{8}\right)\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\mathbf{\hat{x}} + a\left(x_3 + \frac{1}{2}\right)\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(8d)	Mn II
$\mathbf{B_{11}}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \left(x_4 + \frac{1}{8}\right)\,\mathbf{a}_2 + \left(x_4 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_4\,\mathbf{\hat{x}} + \frac{1}{4}a\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(8d)	Sn I
$\mathbf{B_{12}}$	=	$\frac{7}{8}\,\mathbf{a}_1 - \left(x_4 - \frac{1}{8}\right)\,\mathbf{a}_2 - \left(x_4 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_4\,\mathbf{\hat{x}} + \frac{3}{4}a\,\mathbf{\hat{y}} + \frac{1}{8}c\,\mathbf{\hat{z}}$	(8d)	Sn I
$\mathbf{B_{13}}$	=	$-\left(x_4 - \frac{7}{8}\right)\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 - \left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\mathbf{\hat{x}} - a\left(x_4 - \frac{1}{2}\right)\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(8d)	Sn I
$\mathbf{B_{14}}$	=	$\left(x_4 + \frac{7}{8}\right)\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\mathbf{\hat{x}} + a\left(x_4 + \frac{1}{2}\right)\,\mathbf{\hat{y}} + \frac{3}{8}c\,\mathbf{\hat{z}}$	(8d)	Sn I

References

[1] P. Vir, N. Kumar, H. Borrmann, B. Jamijansuren, G. Kreiner, C. Shekhar, and C. Felser, *Tetragonal Superstructure of the Antiskyrmion Hosting Heusler Compound* $Mn_{1.4}PtSn$, Chem. Mater. **31**, 5876–5880 (2019), doi:10.1021/acs.chemmater.9b02013.