Mavlyanovite (Mn_5Si_3, $D8_8$) Structure: A5B3_hP16_193_dg_g-001

This structure originally had the label `A5B3_hP16_193_dg_g`. Calls to that address will be redirected here.

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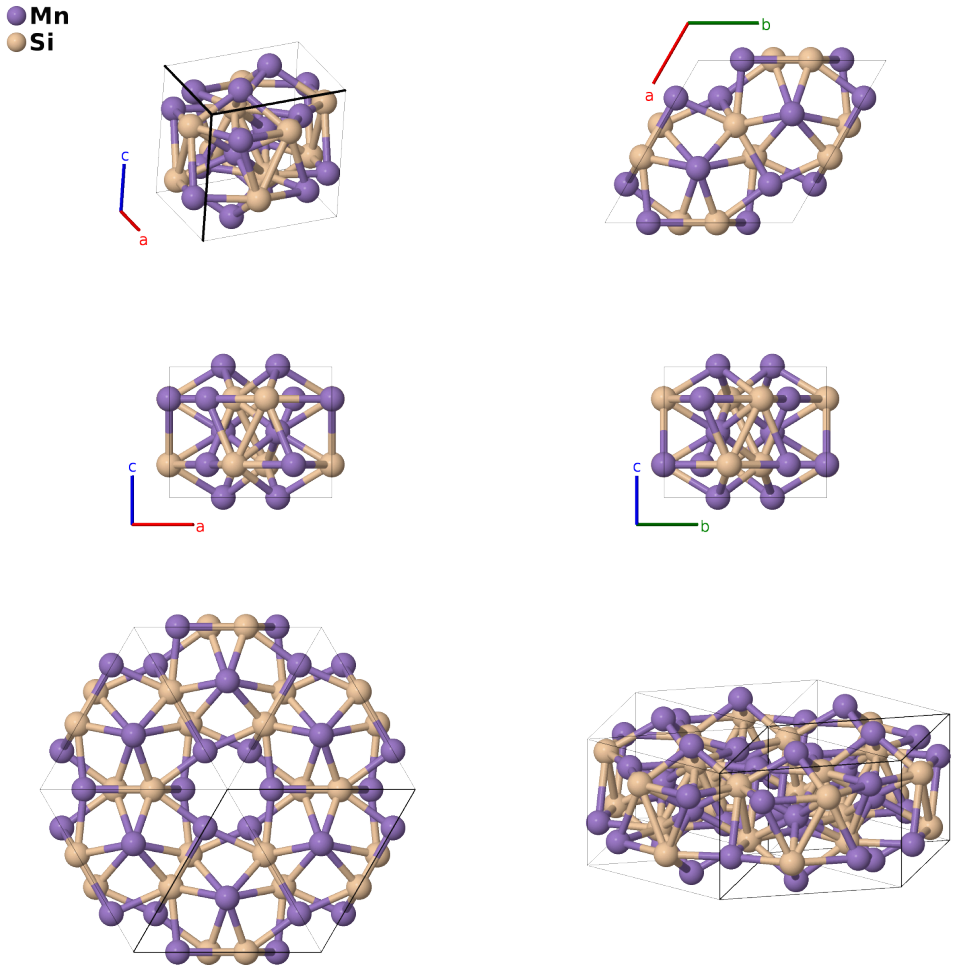
https://aflow.org/p/AQ0J

https://aflow.org/p/A5B3_hP16_193_dg_g-001



Prototype	Mn_5Si_3
AFLOW prototype label	A5B3_hP16_193_dg_g-001
***Strukturbericht* designation**	$D8_8$
Mineral name	mavlyanovite
ICSD	24359
Pearson symbol	hP16
Space group number	193

Space group symbol $P6_3/mcm$

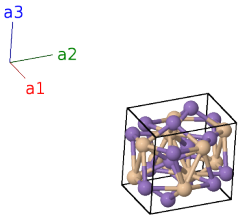
AFLOW prototype command `aflow --proto=A5B3_hP16_193_dg_g-001 --params=`$a, c/a, x_2, x_3$

Other compounds with this structure

Ce_5Ge_3, Ce_5Pb_3, Ce_5Sb_3, Dy_5Ge_3, Dy_5Sb_3, Er_5Si_3, Fe_5Si_3 (HT), Gd_5Ge_3, Gd_5Sb_3, Hf_5Ga_3, Hf_5Ge_3, Hf_5Si_3, Hf_5Sn_3, Ho_5Sb_3, Ho_5Sn_3, La_5Ge_3, La_5Pb_3, La_5Sb_3, Lu_5Si_3, Mg_5Hg_3, Mn_5Ge_3, Mn_5Si_3, Mo_5Si_3, Nb_5Ge_3, Nb_5Si_3, Nd_5Sb_3, Pr_5Sb_3, Sc_5Ga_3, Sc_5Ge_3, Sc_5Pb_3, Sc_5Si_3, Sc_5Sn_3, Ta_5Si_3, Tb_5Sb_3, Ti_5Ga_3, Ti_5Ge_3, Ti_5P_3, Ti_5Si_3, Ti_5Sn_3, U_5Ge_3, V_5Ga_3, V_5Ge_3, V_5Si_3, W_5Si_3, Y_5Ga_3, Y_5Ge_3, Y_5Pb_3, Y_5Si_3, Y_5Sn_3, Yb_5Sb_3, Zr_5Al_3, Zr_5Ga_3, Zr_5Ge_3, Zr_5Pb_3, Zr_5Pt_3, Zr_5Sb_3, Zr_5Si_3, Zr_5Sn_3, $Cr_{5-x-y}Fe_xNb_ySi_3$, $Mn_{5-x}Fe_xSi_3$, $Ti_5Ga_{1.5}Ge_{1.5}$

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(4d)	Mn I
$\mathbf{B_2}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4d)	Mn I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(4d)	Mn I
$\mathbf{B_4}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4d)	Mn I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	Mn II
$\mathbf{B_6}$	=	$x_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	Mn II
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	Mn II
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	Mn II
$\mathbf{B_9}$	=	$-x_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	Mn II
$\mathbf{B_{10}}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	Mn II
$\mathbf{B_{11}}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	Si I
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	Si I
$\mathbf{B_{13}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6g)	Si I
$\mathbf{B_{14}}$	=	$-x_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	Si I
$\mathbf{B_{15}}$	=	$-x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	Si I
$\mathbf{B_{16}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6g)	Si I

References

[1] B. Aronson, *A Note on the Compositions and Crystal Structures of MnB_2, Mn_3Si, Mn_5Si_3, and $FeSi_2$*, Acta Chem. Scand. **14**, 1414–1418 (1960), doi:10.3891/acta.chem.scand.14-1414.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.