$MnGa_2Sb_2$ Structure: A2BC2_oI20_45_c_a_c-001

This structure originally had the label `A2BC2_oI20_45_c_b_c`. Calls to that address will be redirected here.

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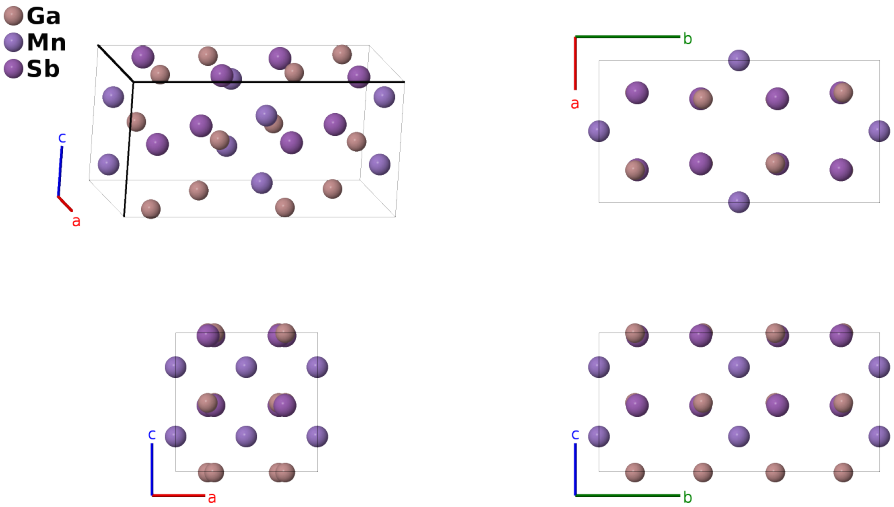
https://aflow.org/p/LNLG

https://aflow.org/p/A2BC2_oI20_45_c_a_c-001

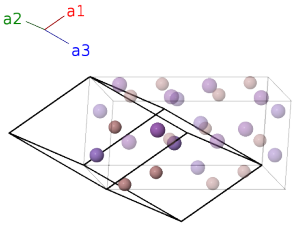


Prototype	Ga_2MnSb_2
AFLOW prototype label	A2BC2_oI20_45_c_a_c-001
ICSD	none
Pearson symbol	oI20
Space group number	45
Space group symbol	$Iba2$
AFLOW prototype command	`aflow --proto=A2BC2_oI20_45_c_a_c-001 --params=`$a, b/a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3$

- The Mn site has an occupation of 0.9365.
- We shifted the origin so that the Mn atom is at the (4a) site rather than the (4b) site.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(4a)	Mn I
$\mathbf{B_2}$	=	$\left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Mn I
$\mathbf{B_3}$	=	$(y_2 + z_2)\,\mathbf{a}_1 + (x_2 + z_2)\,\mathbf{a}_2 + (x_2 + y_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8c)	Ga I
$\mathbf{B_4}$	=	$-(y_2 - z_2)\,\mathbf{a}_1 - (x_2 - z_2)\,\mathbf{a}_2 - (x_2 + y_2)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8c)	Ga I
$\mathbf{B_5}$	=	$\left(-y_2 + z_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + z_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_2 - y_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Ga I
$\mathbf{B_6}$	=	$\left(y_2 + z_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_2 + z_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - (x_2 - y_2)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Ga I
$\mathbf{B_7}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + (x_3 + y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8c)	Sb I
$\mathbf{B_8}$	=	$-(y_3 - z_3)\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - (x_3 + y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8c)	Sb I
$\mathbf{B_9}$	=	$\left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_3 - y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Sb I
$\mathbf{B_{10}}$	=	$\left(y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - (x_3 - y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	Sb I

References

[1] W. Sakakibara, Y. Hayashi, and H. Takizawa, *$MnGa_2Sb_2$, a new ferromagnetic compound synthesized under high pressure*, J. Ceram. Soc. Jpn. **117**, 72–75 (2009), doi:10.2109/jcersj2.117.72.

Found in

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