$Sr_2Mn_3As_2O_2$ Structure: A2B3C2D2_tI18_139_e_ad_c_e-001

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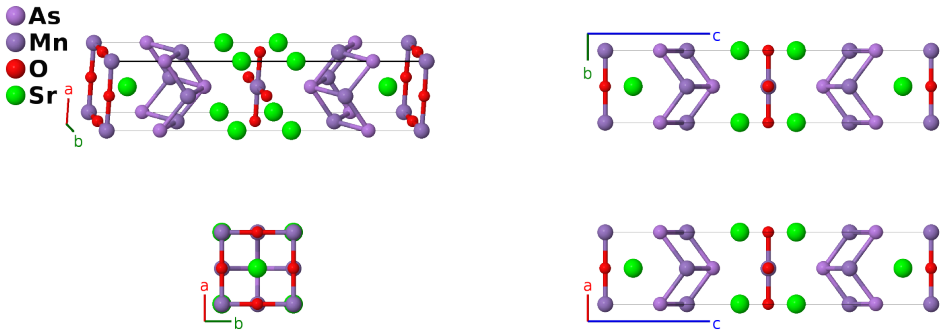
https://aflow.org/p/A2B3C2D2_tI18_139_e_ad_c_e-001



Prototype	$As_2Mn_3O_2Sr_2$
AFLOW prototype label	A2B3C2D2_tI18_139_e_ad_c_e-001
ICSD	81798
Pearson symbol	tI18
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A2B3C2D2_tI18_139_e_ad_c_e-001 --params=`$a, c/a, z_4, z_5$

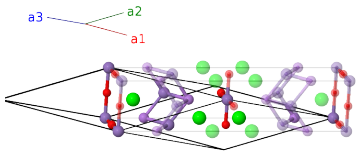
Other compounds with this structure

$La_2O_3Fe_2S_2$, $La_2O_3Fe_2Se_2$, $Sr_2(Mn_2Cu)As_2O_2$, $Sr_2(MnZn_2)As_2O_2$, $Sr_2Mn_3Sb_2O_2$

- We use the data taken by (Brock, 1996) at 275K.

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	(2a)	Mn I

$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(4c)	O I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4c)	O I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Mn II
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Mn II
$\mathbf{B_6}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	As I
$\mathbf{B_7}$	=	$-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	As I
$\mathbf{B_8}$	=	$z_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2$	=	$cz_5\,\hat{\mathbf{z}}$	(4e)	Sr I
$\mathbf{B_9}$	=	$-z_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2$	=	$-cz_5\,\hat{\mathbf{z}}$	(4e)	Sr I

References

[1] S. L. Brock, N. P. Raju, J. E. Greedan, and S. M. Kauzlarich, *The magnetic structures of the mixed layer pnictide oxide compounds $Sr_2Mn_3Pn_2O_2$ (Pn = As, Sb)*, J. Alloys Compd. **237**, 9–19 (1996), doi:10.1016/0925-8388(95)02066-7.

Found in

[1] R. Nath, V. O. Garlea, A. I. Goldman, and D. C. Johnston, *Synthesis, structure, and properties of tetragonal $Sr_2M_3As_2O_2$ (M_3=Mn_3, Mn_2Cu, and $MnZn_2$) compounds containing alternating*, Phys. Rev. B **81**, 224513 (2010), doi:10.1103/PhysRevB.81.224513.