

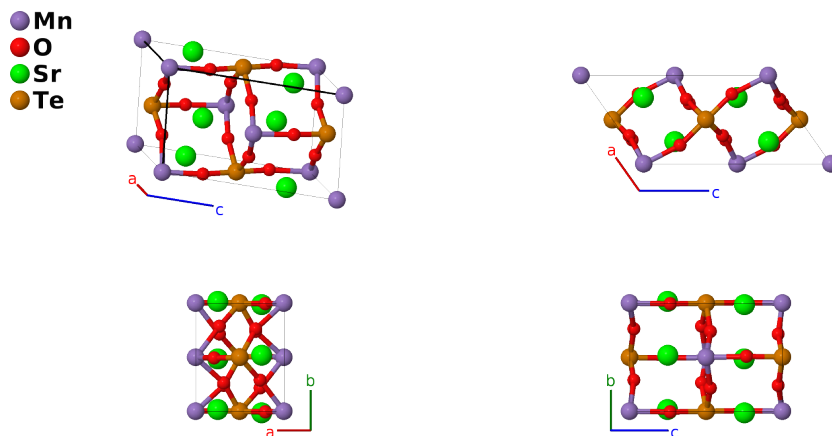
Sr₂MnTeO₆ Structure: AB6C2D_mP20_14_a_3e_e_b-001

This structure originally had the label AB6C2D_mP20_14_a_3e_e_d. Calls to that address will be redirected here.

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<https://aflow.org/p/QXEE>

https://aflow.org/p/AB6C2D_mP20_14_a_3e_e_b-001



Prototype	MnO ₆ Sr ₂ Te
AFLOW prototype label	AB6C2D_mP20_14_a_3e_e_b-001
ICSD	none
Pearson symbol	mP20
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	<pre>aflow --proto=AB6C2D_mP20_14_a_3e_e_b-001 --params=a,b/a,c/a,β,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6</pre>

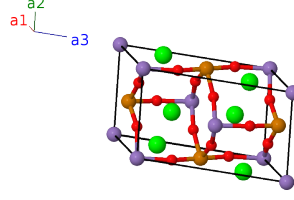
Other compounds with this structure

Ba₂LaIrO₆, Ba₂RuO₆, Ba₂LuIrO₆, Ba₂NaIrO₆, Ba₂YIrO₆, Cs₂RbDyF₆, Dy₂MnNiO₆, Eu₂MgIrO₆, Eu₂MnNiO₆, Eu₂ZnIrO₆, Gd₂MgIrO₆, Gd₂MnNiO₆, Gd₂ZnIrO₆, Ho₂MnNiO₆, La₂MnCoO₆, La₂MnFeO₆, La₂MnNiO₆, Lu₂MnNiO₆, Nd₂MgIrO₆, Nd₂MnNiO₆, Nd₂ZnIrO₆, Pr₂MgIrO₆, Pr₂MnNiO₆, Pr₂ZnIrO₆, Sm₂MgIrO₆, Sm₂MnNiO₆, Sm₂ZnIrO₆, Sr₂CaIrO₆, Sr₂CdTeO₆, Sr₂ErRuO₆, Sr₂InIrO₆, Sr₂LuIrO₆, Sr₂MgIrO₆, Sr₂MnReO_{5.8}, Sr₂ScIrO₆, Sr₂TmRuO₆, Sr₂YIrO₆, Sr₂YbRuO₆, Ca(Ca_{1/2}Nd_{1/2})₂NbO₆

- This is the ground state structure of the double perovskite Sr₂MnTeO₆. Above 250°C it transforms into the Sr₂NiTeO₆ structure. Above 550°C it transforms into the Sr₂NiWO₆ structure, and above 675°C it transforms into the cubic perovskite $E2_1$ structure. (Ortega-San Martin, 2004).
- (Ortega-San Martin, 2004) give the structure in the $P2_1/n$ setting of space group #14. We used findsym to transform this to the standard $P2_1/c$ setting, which uses a different set of basis vectors.

Simple Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(2a)	Mn I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \cos \beta \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$	(2a)	Mn I
\mathbf{B}_3	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(2b)	Te I
\mathbf{B}_4	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} (a + c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$	(2b)	Te I
\mathbf{B}_5	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	O I
\mathbf{B}_6	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O I
\mathbf{B}_7	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	O I
\mathbf{B}_8	$x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O I
\mathbf{B}_9	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	O II
\mathbf{B}_{10}	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O II
\mathbf{B}_{11}	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	O II
\mathbf{B}_{12}	$x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O II
\mathbf{B}_{13}	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4e)	O III
\mathbf{B}_{14}	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O III
\mathbf{B}_{15}	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4e)	O III
\mathbf{B}_{16}	$x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	O III
\mathbf{B}_{17}	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4e)	Sr I
\mathbf{B}_{18}	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_6 + c(z_6 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Sr I
\mathbf{B}_{19}	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4e)	Sr I
\mathbf{B}_{20}	$x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	Sr I

References

- [1] L. O.-S. Martin, J. P. Chapman, E. Hernández-Bocanegra, M. Insausti, M. I. Arriortua, and T. Rojo, *Structural phase transitions in the ordered double perovskite Sr_2MnTeO_6* , J. Phys.: Condens. Matter **16**, 3879–3888 (2004), doi:10.1088/0953-8984/16/23/008.