

SrMn₇O₁₂ Structure:

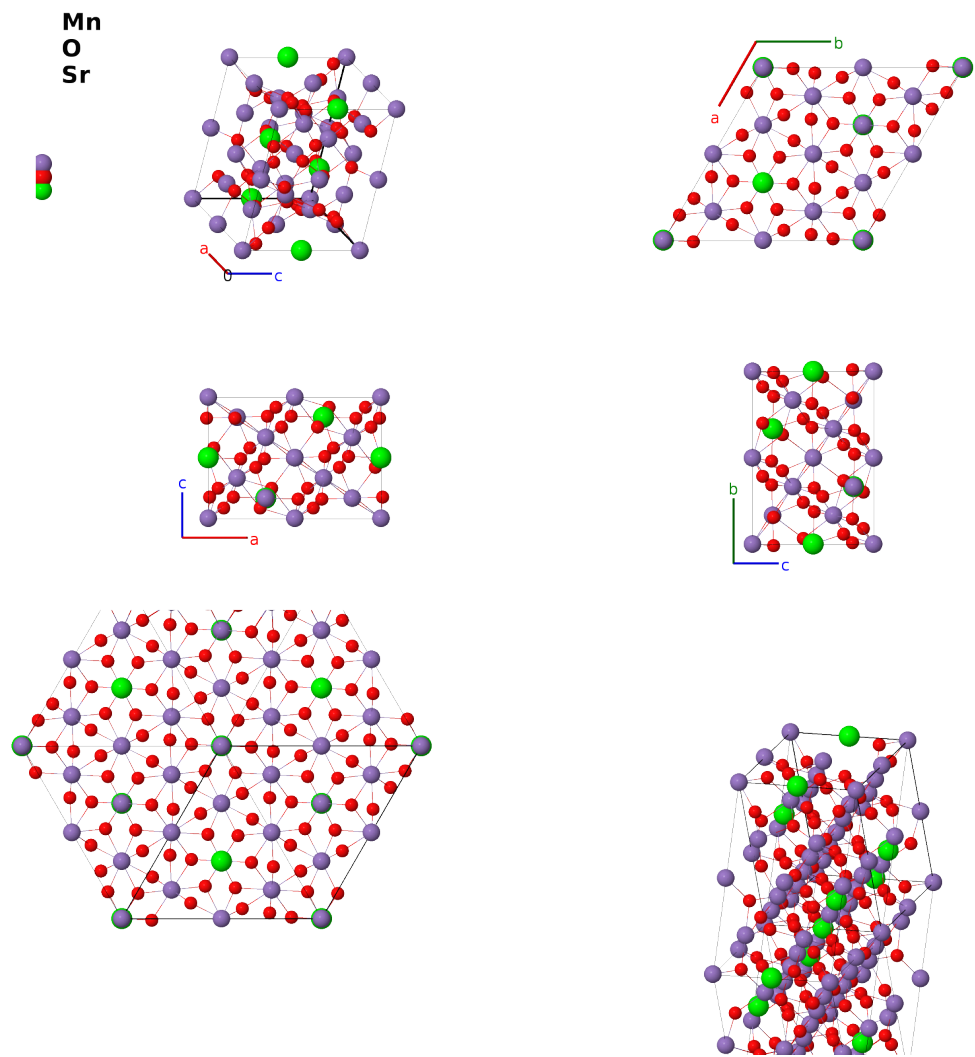
A7B12C_hR20_148_ade_2f_b-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/5YFD>

https://aflow.org/prototype-encyclopedia/A7B12C_hR20_148_ade_2f_b-001



Prototype	Mn ₇ O ₁₂ Sr
AFLOW prototype label	A7B12C_hR20_148_ade_2f_b-001
ICSD	252386
CCDC	1717711
Pearson symbol	hR20

Space group number	148
Space group symbol	$R\bar{3}$
AFLOW prototype command	<code>aflow --proto=A7B12C_hR20_148_ade_2f_b-001</code> <code>--params=a, c/a, x₅, y₅, z₅, x₆, y₆, z₆</code>

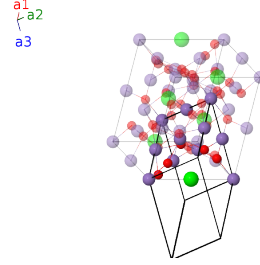
Other compounds with this structure

CaMn₇O₁₂, CdMn₇O₁₂, PbMn₇O₁₂, PrMn₇O₁₂

- We use the data for SrMn₇O₁₂ taken at 295K. Below 265K it undergoes an incommensurate structural transition. (Belik, 2016)
- Some authors use CaMn₇O₁₂ as the prototype.
- At high temperatures CaMn₇O₁₂, PbMn₇O₁₂ and PrMn₇O₇ transform into the NaMn₇O₁₂ structure.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(1a)	Mn I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	(1b)	Sr I
$\mathbf{B}_3$	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3d)	Mn II
$\mathbf{B}_4$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3d)	Mn II
$\mathbf{B}_5$	$\frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3d)	Mn II
$\mathbf{B}_6$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3e)	Mn III
$\mathbf{B}_7$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3e)	Mn III
$\mathbf{B}_8$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3e)	Mn III
$\mathbf{B}_9$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B}_{10}$	$z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B}_{11}$	$y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B}_{12}$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B}_{13}$	$-z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	O I

$$\begin{aligned}
\mathbf{B}_{14} &= -y_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3 &= \frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}} &(6f) &\quad \text{O I} \\
\mathbf{B}_{15} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= \frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) &\quad \text{O II} \\
\mathbf{B}_{16} &= z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3 &= -\frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) &\quad \text{O II} \\
\mathbf{B}_{17} &= y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3 &= -\frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) &\quad \text{O II} \\
\mathbf{B}_{18} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) &\quad \text{O II} \\
\mathbf{B}_{19} &= -z_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - y_6 \mathbf{a}_3 &= \frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) &\quad \text{O II} \\
\mathbf{B}_{20} &= -y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 - x_6 \mathbf{a}_3 &= \frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) &\quad \text{O II}
\end{aligned}$$

References

- [1] A. A. Belik, Y. S. Glazkova, Y. Katsuya, M. Tanaka, A. V. Sobolev, and I. A. Presniakov, *Low-Temperature Structural Modulations in $\text{CdMn}_7\text{O}_{12}$, $\text{CaMn}_7\text{O}_{12}$, $\text{SrMn}_7\text{O}_{12}$, and $\text{PbMn}_7\text{O}_{12}$ Perovskites Studied by Synchrotron X-ray Powder Diffraction and Mössbauer Spectroscopy*, J. Phys. Chem. C **120**, 8278–8288 (2016), doi:10.1021/acs.jpcc.6b01649.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.