# $SrMn_7O_{12}$ Structure: A7B12C_hR20_148_ade_2f_b-001

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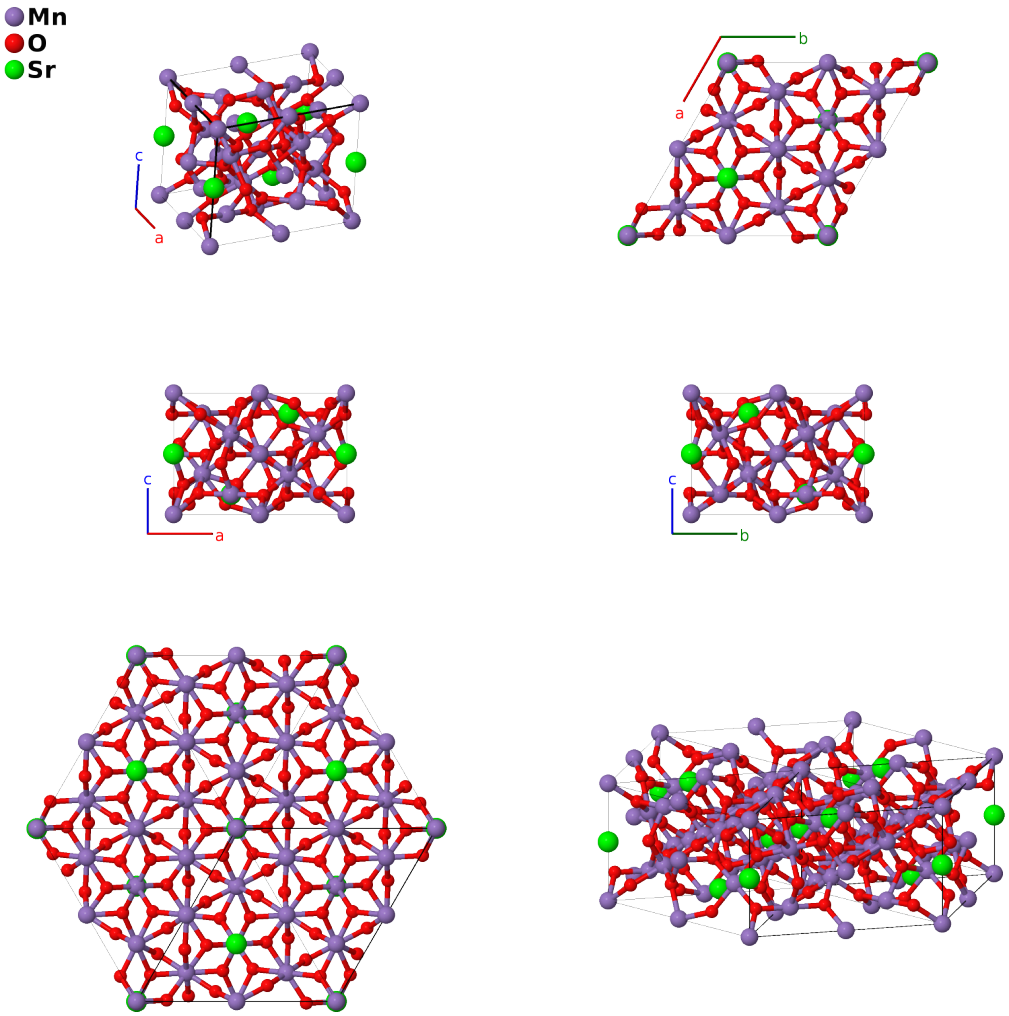
https://aflow.org/p/5YFD

https://aflow.org/p/A7B12C_hR20_148_ade_2f_b-001



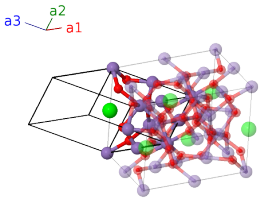

| | |
|---|---|
| **Prototype** | $Mn_7O_{12}Sr$ |
| **AFLOW prototype label** | A7B12C_hR20_148_ade_2f_b-001 |
| **ICSD** | 252386 |
| **Pearson symbol** | hR20 |
| **Space group number** | 148 |
| **Space group symbol** | $R\bar{3}$ |
| **AFLOW prototype command** | `aflow --proto=A7B12C_hR20_148_ade_2f_b-001 --params=`$a, c/a, x_5, y_5, z_5, x_6, y_6, z_6$ |

**Other compounds with this structure**
$CaMn_7O_{12}$, $CdMn_7O_{12}$, $PbMn_7O_{12}$

- We use the data for $SrMn_7O_{12}$ taken at 295K. Below 265K it undergoes an incommensurate structural transition. (Belik, 2016)
- Some authors use $CaMn_7O_{12}$ as the prototype.
- At high temperatures $CaMn_7O_{12}$ and $PbMn_7O_{12}$ transform into the $NaMn_7O_{12}$ structure.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

**Rhombohedral primitive vectors**

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$




**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 |
| $\mathbf{B_{14}}$ | = | $-y_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_5 - y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_5 + y_5 - 2z_5)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$ | (6f) | 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) | 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) | 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) | 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) | 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) | 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) | O II |

## References


[1] A. A. Belik, Y. S. Glazkova, Y. Katsuya, M. Tanaka, A. V. Sobolev, and I. A. Presniakov, *Low-Temperature Structural Modulations in $CdMn_7O_{12}$, $CaMn_7O_{12}$, $SrMn_7O_{12}$, and $PbMn_7O_{12}$ 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.