# $NaMn_7O_{12}$ Structure: A7BC12_cI40_204_bc_a_g-001

This structure originally had the label `A7BC12_cI40_204_bc_a_g`. Calls to that address will be redirected here.

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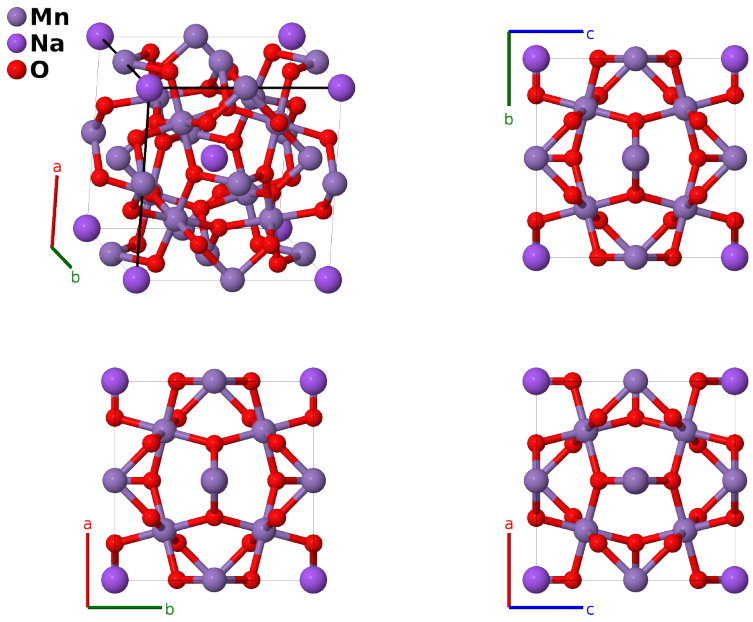
https://aflow.org/p/M5NA

https://aflow.org/p/A7BC12_cI40_204_bc_a_g-001



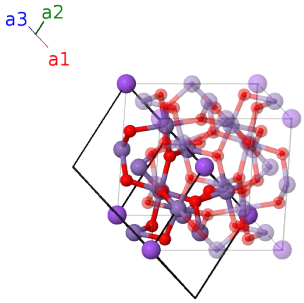

| | |
|---|---|
| **Prototype** | $Mn_7NaO_{12}$ |
| **AFLOW prototype label** | A7BC12_cI40_204_bc_a_g-001 |
| **ICSD** | 154189 |
| **Pearson symbol** | cI40 |
| **Space group number** | 204 |
| **Space group symbol** | $Im\bar{3}$ |
| **AFLOW prototype command** | `aflow --proto=A7BC12_cI40_204_bc_a_g-001 --params=`$a, y_4, z_4$ |

**Other compounds with this structure**
$SrMn_7O_{12}$

- This is a double perovskite structure. It is stable above 3GBar and above room temperature, but is metastable under ambient conditions (Gilioli 2005ab). The actual composition of the measured sample is $Na_{0.95}Mn_{7.05}O_{12}$, with the excess manganese displacing some of the sodium atoms on the (2a) site.
- The (6b) and (6c) sites may be populated by two species of atoms. In that case we get the quaternary form of this structure, prototype $CaCu_3Mn_4O_{12}$.

## Body-centered Cubic primitive vectors

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




## Basis vectors

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (2a) | Na I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}}$ | (6b) | Mn I |
| $\mathbf{B_3}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}}$ | (6b) | Mn I |
| $\mathbf{B_4}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$ | = | $\frac{1}{2}a\,\hat{\mathbf{z}}$ | (6b) | Mn I |
| $\mathbf{B_5}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$ | (8c) | Mn II |
| $\mathbf{B_6}$ | = | $\frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - \frac{1}{4}a\,\hat{\mathbf{z}}$ | (8c) | Mn II |
| $\mathbf{B_7}$ | = | $\frac{1}{2}\,\mathbf{a}_2$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$ | (8c) | Mn II |
| $\mathbf{B_8}$ | = | $\frac{1}{2}\,\mathbf{a}_1$ | = | $-\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$ | (8c) | Mn II |
| $\mathbf{B_9}$ | = | $(y_4 + z_4)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$ | = | $ay_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$ | (24g) | O I |
| $\mathbf{B_{10}}$ | = | $-(y_4 - z_4)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$ | = | $-ay_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$ | (24g) | O I |
| $\mathbf{B_{11}}$ | = | $(y_4 - z_4)\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$ | = | $ay_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}}$ | (24g) | O I |
| $\mathbf{B_{12}}$ | = | $-(y_4 + z_4)\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$ | = | $-ay_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}}$ | (24g) | O I |
| $\mathbf{B_{13}}$ | = | $y_4\,\mathbf{a}_1 + (y_4 + z_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $az_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{z}}$ | (24g) | O I |
| $\mathbf{B_{14}}$ | = | $-y_4\,\mathbf{a}_1 - (y_4 - z_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $az_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{z}}$ | (24g) | O I |
| $\mathbf{B_{15}}$ | = | $y_4\,\mathbf{a}_1 + (y_4 - z_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$ | = | $-az_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{z}}$ | (24g) | O I |
| $\mathbf{B_{16}}$ | = | $-y_4\,\mathbf{a}_1 - (y_4 + z_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$ | = | $-az_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{z}}$ | (24g) | O I |
| $\mathbf{B_{17}}$ | = | $z_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + (y_4 + z_4)\,\mathbf{a}_3$ | = | $ay_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}}$ | (24g) | O I |
| $\mathbf{B_{18}}$ | = | $z_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - (y_4 - z_4)\,\mathbf{a}_3$ | = | $-ay_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}}$ | (24g) | O I |
| $\mathbf{B_{19}}$ | = | $-z_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + (y_4 - z_4)\,\mathbf{a}_3$ | = | $ay_4\,\hat{\mathbf{x}} - az_4\,\hat{\mathbf{y}}$ | (24g) | O I |
| $\mathbf{B_{20}}$ | = | $-z_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - (y_4 + z_4)\,\mathbf{a}_3$ | = | $-ay_4\,\hat{\mathbf{x}} - az_4\,\hat{\mathbf{y}}$ | (24g) | O I |

## References


[1] E. Gilioli, G. Calestani, F. Licci, A. Gauzzi, F. Bolzoni, A. Prodi, and M. Marezio, *$P-T$ phase diagram and single crystal structural refinement of $NaMn_7O_{12}$*, Solid State Sci. **7**, 746–752 (2005), doi:10.1016/j.solidstatesciences.2004.11.020.


## Found in


[1] E. Gilioli, F. Licci, G. Calestani, A. Prodi, A. Gauzzi, and G. Salviati, *Crystal growth and structural refinement of $NaMn_7O_{12}$*, Crys. Res. Technol. **40**, 1072–1075 (2005), doi:10.1002/crat.200410489.