

PrMn₇O₁₂ Structure:

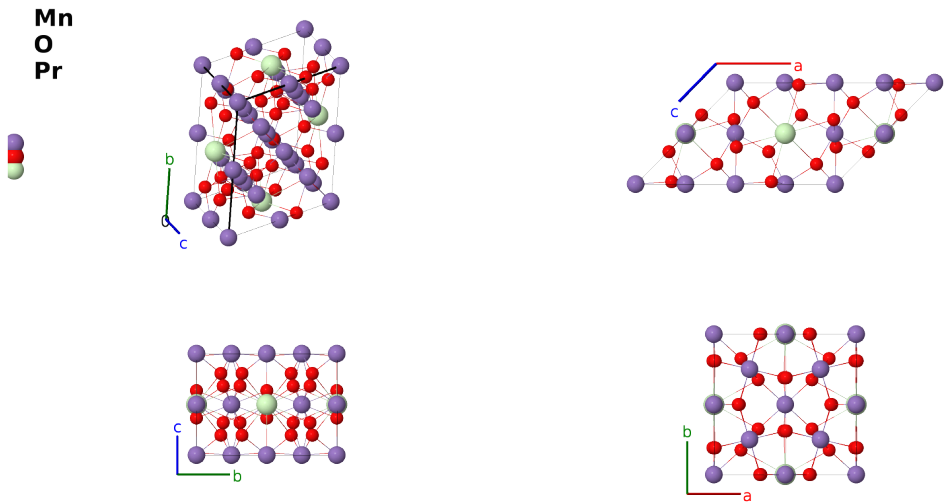
A7B12C_mC40_12_abcef_2i2j_d-001

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<https://aflow.org/prototype-encyclopedia/8GW0>

https://aflow.org/prototype-encyclopedia/A7B12C_mC40_12_abcef_2i2j_d-001



Prototype	Mn ₇ O ₁₂ Pr
AFLOW prototype label	A7B12C_mC40_12_abcef_2i2j_d-001
ICSD	163258
CCDC	1679425
Pearson symbol	mC40
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<pre>aflow --proto=A7B12C_mC40_12_abcef_2i2j_d-001 --params=a, b/a, c/a, β, x_7, z_7, x_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}</pre>

Other compounds with this structure

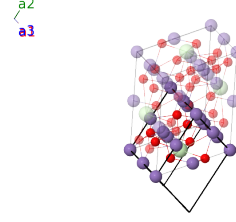
BiMn₇O₁₂, CeMn₇O₁₂, EuMn₇O₁₂, LaMn₇O₁₂, NaMn₇O₁₂, NdMn₇O₁₂, SmMn₇O₁₂, SmMn₇O₁₂, YMn₇O₁₂

- The rare-earth quadruple perovskite manganites, RMn_7O_{12} undergo a variety of transformations as they cool from the high temperature cubic $NaMn_7O_{12}$ form. This $PrMn_7O_{12}$ structure is often the first phase transition after cooling. (Mezzadri, 2009; Okamoto, 2010; Johnson 2018; Behr, 2023).
- (Mezzadri, 2009) found two slightly different structures for this phase depending “on the synthesis conditions.” We use their monoclinic (I) structure here.

- This structure is exclusively reported in the *base*-centered monoclinic $I2/m$ setting of space group #12, as this results in a conventional unit cell that is nearly cubic. AFLOW translates this into the standard *body*-centered monoclinic $C2/m$ setting.

Base-centered Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	Mn I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}}$	Mn II
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	Mn III
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}(a + c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	Pr I
$\mathbf{B}_5$	$=$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}}$	Mn IV
$\mathbf{B}_6$	$=$	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}}$	Mn IV
$\mathbf{B}_7$	$=$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\left(\frac{a}{4} + \frac{c \cos \beta}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	Mn V
$\mathbf{B}_8$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\left(\frac{a}{4} + \frac{c \cos \beta}{2}\right) \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	Mn V
$\mathbf{B}_9$	$=$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + cz_7 \sin \beta \hat{\mathbf{z}}$	O I
$\mathbf{B}_{10}$	$=$	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - cz_7 \sin \beta \hat{\mathbf{z}}$	O I
$\mathbf{B}_{11}$	$=$	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + cz_8 \sin \beta \hat{\mathbf{z}}$	O II
$\mathbf{B}_{12}$	$=$	$-x_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - cz_8 \sin \beta \hat{\mathbf{z}}$	O II
$\mathbf{B}_{13}$	$=$	$(x_9 - y_9) \mathbf{a}_1 + (x_9 + y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	O III
$\mathbf{B}_{14}$	$=$	$-(x_9 + y_9) \mathbf{a}_1 - (x_9 - y_9) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	O III
$\mathbf{B}_{15}$	$=$	$-(x_9 - y_9) \mathbf{a}_1 - (x_9 + y_9) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	O III
$\mathbf{B}_{16}$	$=$	$(x_9 + y_9) \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	O III
$\mathbf{B}_{17}$	$=$	$(x_{10} - y_{10}) \mathbf{a}_1 + (x_{10} + y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	O IV
$\mathbf{B}_{18}$	$=$	$-(x_{10} + y_{10}) \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	O IV
$\mathbf{B}_{19}$	$=$	$-(x_{10} - y_{10}) \mathbf{a}_1 - (x_{10} + y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	O IV
$\mathbf{B}_{20}$	$=$	$(x_{10} + y_{10}) \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	O IV

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Found in

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