Triclinic $BiMn_7O_{12}$ Structure: AB7C12_aP20_1_a_7a_12a-001

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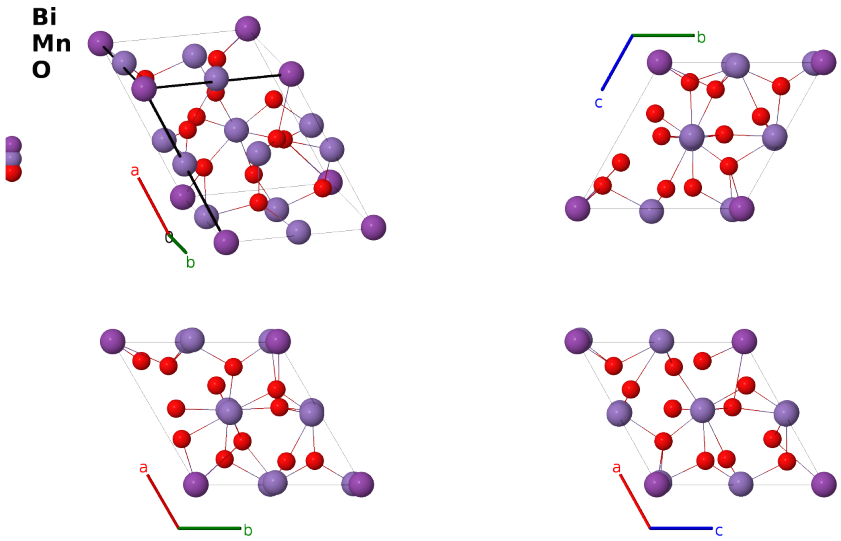
https://aflow.org/prototype-encyclopedia/UR03

https://aflow.org/prototype-encyclopedia/AB7C12_aP20_1_a_7a_12a-001



Prototype	$BiMn_7O_{12}$
AFLOW prototype label	AB7C12_aP20_1_a_7a_12a-001
ICSD	24447
CCDC	1527727
Pearson symbol	aP20
Space group number	1
Space group symbol	$P1$
AFLOW prototype command	`aflow --proto=AB7C12_aP20_1_a_7a_12a-001 --params=`$a, b/a, c/a, \alpha, \beta, \gamma, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}$

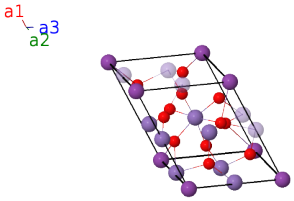
- As with all rare-earth quadruple perovskite manganites (RMn_7O_{12}) undergoes a series of phase transitions with increasing temperature (Behr, 2023):
  - Below 290K it is in this triclinic $BiMn_7O_{12}$ structure.
  - Between 290 and 460K it is in the monoclinic $BiMn_7O_{12}$ structure.
  - Between 460 and 608K it is in the monoclinic $PrMn_7O_{12}$ structure.

– Above 608K it is in the parent cubic $NaMn_7O_{12}$ structure.

- The primitive unit cell for this structure is nearly body-centered cubic ($a \approx b \approx c, \alpha \approx \beta \approx \gamma \approx \cos^{-1}(-1/3)$, and (Sławiński, 2017) present it in the body-centered $I1$ setting of space group #1. The ICSD entry is transformed into the standard $P1$ setting, so we use that data.
- The location of the origin for triclinic space groups is completely arbitrary. (Sławiński, 2017) choose to put the bismuth atom at the origin.

Triclinic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= a\,\hat{\mathbf{x}} \\
\mathbf{a_2} &= b\cos\gamma\,\hat{\mathbf{x}} + b\sin\gamma\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c_x\,\hat{\mathbf{x}} + c_y\,\hat{\mathbf{y}} + c_z\,\hat{\mathbf{z}} \\
c_x &= c\cos\beta \\
c_y &= c(\cos\alpha - \cos\beta\cos\gamma)/\sin\gamma \\
c_z &= \sqrt{c^2 - c_x^2 - c_y^2}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + by_1\cos\gamma + c_x z_1)\,\hat{\mathbf{x}} + (by_1\sin\gamma + c_y z_1)\,\hat{\mathbf{y}} + c_z z_1\,\hat{\mathbf{z}}$	(1a)	Bi I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + by_2\cos\gamma + c_x z_2)\,\hat{\mathbf{x}} + (by_2\sin\gamma + c_y z_2)\,\hat{\mathbf{y}} + c_z z_2\,\hat{\mathbf{z}}$	(1a)	Mn I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + by_3\cos\gamma + c_x z_3)\,\hat{\mathbf{x}} + (by_3\sin\gamma + c_y z_3)\,\hat{\mathbf{y}} + c_z z_3\,\hat{\mathbf{z}}$	(1a)	Mn II
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + by_4\cos\gamma + c_x z_4)\,\hat{\mathbf{x}} + (by_4\sin\gamma + c_y z_4)\,\hat{\mathbf{y}} + c_z z_4\,\hat{\mathbf{z}}$	(1a)	Mn III
$\mathbf{B_5}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + by_5\cos\gamma + c_x z_5)\,\hat{\mathbf{x}} + (by_5\sin\gamma + c_y z_5)\,\hat{\mathbf{y}} + c_z z_5\,\hat{\mathbf{z}}$	(1a)	Mn IV
$\mathbf{B_6}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + by_6\cos\gamma + c_x z_6)\,\hat{\mathbf{x}} + (by_6\sin\gamma + c_y z_6)\,\hat{\mathbf{y}} + c_z z_6\,\hat{\mathbf{z}}$	(1a)	Mn V
$\mathbf{B_7}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + by_7\cos\gamma + c_x z_7)\,\hat{\mathbf{x}} + (by_7\sin\gamma + c_y z_7)\,\hat{\mathbf{y}} + c_z z_7\,\hat{\mathbf{z}}$	(1a)	Mn VI
$\mathbf{B_8}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + by_8\cos\gamma + c_x z_8)\,\hat{\mathbf{x}} + (by_8\sin\gamma + c_y z_8)\,\hat{\mathbf{y}} + c_z z_8\,\hat{\mathbf{z}}$	(1a)	Mn VII
$\mathbf{B_9}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + by_9\cos\gamma + c_x z_9)\,\hat{\mathbf{x}} + (by_9\sin\gamma + c_y z_9)\,\hat{\mathbf{y}} + c_z z_9\,\hat{\mathbf{z}}$	(1a)	O I
$\mathbf{B_{10}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + by_{10}\cos\gamma + c_x z_{10})\,\hat{\mathbf{x}} + (by_{10}\sin\gamma + c_y z_{10})\,\hat{\mathbf{y}} + c_z z_{10}\,\hat{\mathbf{z}}$	(1a)	O II
$\mathbf{B_{11}}$	=	$x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11} + by_{11}\cos\gamma + c_x z_{11})\,\hat{\mathbf{x}} + (by_{11}\sin\gamma + c_y z_{11})\,\hat{\mathbf{y}} + c_z z_{11}\,\hat{\mathbf{z}}$	(1a)	O III
$\mathbf{B_{12}}$	=	$x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$(ax_{12} + by_{12}\cos\gamma + c_x z_{12})\,\hat{\mathbf{x}} + (by_{12}\sin\gamma + c_y z_{12})\,\hat{\mathbf{y}} + c_z z_{12}\,\hat{\mathbf{z}}$	(1a)	O IV
$\mathbf{B_{13}}$	=	$x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$(ax_{13} + by_{13}\cos\gamma + c_x z_{13})\,\hat{\mathbf{x}} + (by_{13}\sin\gamma + c_y z_{13})\,\hat{\mathbf{y}} + c_z z_{13}\,\hat{\mathbf{z}}$	(1a)	O V
$\mathbf{B_{14}}$	=	$x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3$	=	$(ax_{14} + by_{14}\cos\gamma + c_x z_{14})\,\hat{\mathbf{x}} + (by_{14}\sin\gamma + c_y z_{14})\,\hat{\mathbf{y}} + c_z z_{14}\,\hat{\mathbf{z}}$	(1a)	O VI

$$\mathbf{B_{15}} = x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 = (ax_{15} + by_{15}\cos\gamma + c_x z_{15})\,\hat{\mathbf{x}} + (by_{15}\sin\gamma + c_y z_{15})\,\hat{\mathbf{y}} + c_z z_{15}\,\hat{\mathbf{z}} \quad \text{(1a)} \quad \text{O VII}$$

$$\mathbf{B_{16}} = x_{16}\,\mathbf{a}_1 + y_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 = (ax_{16} + by_{16}\cos\gamma + c_x z_{16})\,\hat{\mathbf{x}} + (by_{16}\sin\gamma + c_y z_{16})\,\hat{\mathbf{y}} + c_z z_{16}\,\hat{\mathbf{z}} \quad \text{(1a)} \quad \text{O VIII}$$

$$\mathbf{B_{17}} = x_{17}\,\mathbf{a}_1 + y_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3 = (ax_{17} + by_{17}\cos\gamma + c_x z_{17})\,\hat{\mathbf{x}} + (by_{17}\sin\gamma + c_y z_{17})\,\hat{\mathbf{y}} + c_z z_{17}\,\hat{\mathbf{z}} \quad \text{(1a)} \quad \text{O IX}$$

$$\mathbf{B_{18}} = x_{18}\,\mathbf{a}_1 + y_{18}\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3 = (ax_{18} + by_{18}\cos\gamma + c_x z_{18})\,\hat{\mathbf{x}} + (by_{18}\sin\gamma + c_y z_{18})\,\hat{\mathbf{y}} + c_z z_{18}\,\hat{\mathbf{z}} \quad \text{(1a)} \quad \text{O X}$$

$$\mathbf{B_{19}} = x_{19}\,\mathbf{a}_1 + y_{19}\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3 = (ax_{19} + by_{19}\cos\gamma + c_x z_{19})\,\hat{\mathbf{x}} + (by_{19}\sin\gamma + c_y z_{19})\,\hat{\mathbf{y}} + c_z z_{19}\,\hat{\mathbf{z}} \quad \text{(1a)} \quad \text{O XI}$$

$$\mathbf{B_{20}} = x_{20}\,\mathbf{a}_1 + y_{20}\,\mathbf{a}_2 + z_{20}\,\mathbf{a}_3 = (ax_{20} + by_{20}\cos\gamma + c_x z_{20})\,\hat{\mathbf{x}} + (by_{20}\sin\gamma + c_y z_{20})\,\hat{\mathbf{y}} + c_z z_{20}\,\hat{\mathbf{z}} \quad \text{(1a)} \quad \text{O XII}$$

References

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Found in

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