

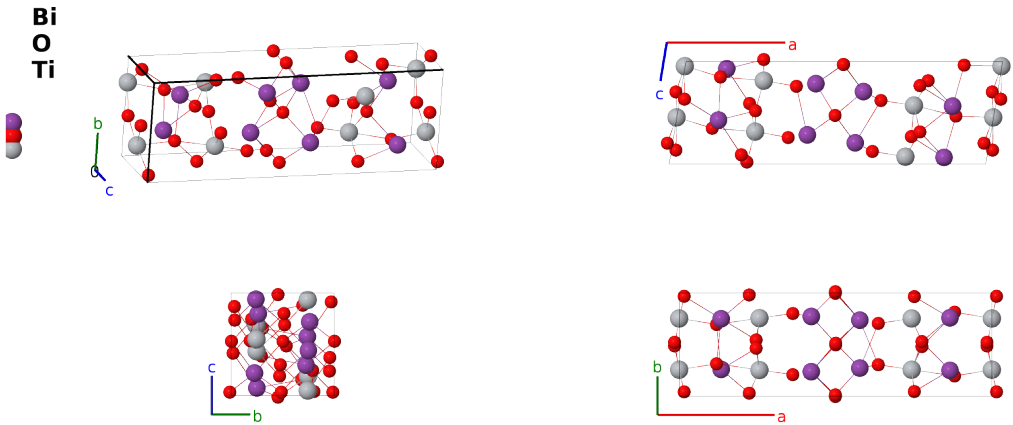
Monoclinic Bi₄Ti₃O₁₂ $m = 3$ Aurivillius Structure: A4B12C3_mP38_7_4a_12a_3a-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/S41T>

https://aflow.org/prototype-encyclopedia/A4B12C3_mP38_7_4a_12a_3a-001



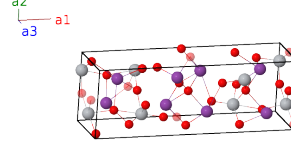
Prototype	Bi ₄ O ₁₂ Ti ₃
AFLOW prototype label	A4B12C3_mP38_7_4a_12a_3a-001
ICSD	38993
CCDC	2228001
Pearson symbol	mP38
Space group number	7
Space group symbol	Pc
AFLOW prototype command	<pre>aflow --proto=A4B12C3_mP38_7_4a_12a_3a-001 --params=a,b/a,c/a,β,x₁,y₁,z₁,x₂,y₂,z₂,x₃,y₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇, y₇,z₇,x₈,y₈,z₈,x₉,y₉,z₉,x₁₀,y₁₀,z₁₀,x₁₁,y₁₁,z₁₁,x₁₂,y₁₂,z₁₂,x₁₃,y₁₃,z₁₃,x₁₄,y₁₄,z₁₄,x₁₅, y₁₅,z₁₅,x₁₆,y₁₆,z₁₆,x₁₇,y₁₇,z₁₇,x₁₈,y₁₈,z₁₈,x₁₉,y₁₉,z₁₉</pre>

- Aurivillius phases are layered tetragonal materials with composition $(\text{Me}'_2\text{O}_2)^{2+}(\text{Me}_{m-1}\text{R}_m\text{O}_{3m+1})^{2-}$ ($\text{Me}_{m-1}\text{Me}'_2\text{R}_m\text{O}_{3(m+1)}$), where Me and Me' are metals and R is a transition metal with a charge of +4 or +5. (Subbaro, 1962)
- (Guo, 2019) describe this system in the base-centered $B1a1$ representation of space group #7. This representation produces a conventional cell that is very close to tetragonal at the cost of doubling the cell size. We used FINDSYM and AFLOW to transform this to the standard Pc setting.

- (Guo, 2019) used a non-standard representation of the $B1a1$ symmetry operations. The ICSD entry for this structure, as well as the companion structure 38988, used the standard representation. As a result, the CIFs from the ICSD entries do not represent the correct structure.
- If we allow an uncertainty of $0.5\text{\AA}$ in the atomic positions this structure becomes virtually identical with the orthorhombic structure found by (Dorrian, 1971).

Simple Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	Bi I
$\mathbf{B}_2$	$x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Bi I
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	Bi II
$\mathbf{B}_4$	$x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Bi II
$\mathbf{B}_5$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	Bi III
$\mathbf{B}_6$	$x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Bi III
$\mathbf{B}_7$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	Bi IV
$\mathbf{B}_8$	$x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Bi IV
$\mathbf{B}_9$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_{10}$	$x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_{11}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B}_{12}$	$x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B}_{13}$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(2a)	O III
$\mathbf{B}_{14}$	$x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O III
$\mathbf{B}_{15}$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(2a)	O IV
$\mathbf{B}_{16}$	$x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_8 + c(z_8 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O IV
$\mathbf{B}_{17}$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(2a)	O V
$\mathbf{B}_{18}$	$x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_9 + c(z_9 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O V
$\mathbf{B}_{19}$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	=	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(2a)	O VI

$$\begin{aligned}
\mathbf{B}_{20} &= x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} ax_{10} + c \left(z_{10} + \frac{1}{2}\right) \cos \beta \\ c \left(z_{10} + \frac{1}{2}\right) \sin \beta \end{pmatrix} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + \quad (2a) \quad \text{O VI} \\
\mathbf{B}_{21} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = \begin{pmatrix} ax_{11} + cz_{11} \cos \beta \\ by_{11} \end{pmatrix} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}} \quad (2a) \quad \text{O VII} \\
\mathbf{B}_{22} &= x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} ax_{11} + c \left(z_{11} + \frac{1}{2}\right) \cos \beta \\ c \left(z_{11} + \frac{1}{2}\right) \sin \beta \end{pmatrix} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + \quad (2a) \quad \text{O VII} \\
\mathbf{B}_{23} &= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 = \begin{pmatrix} ax_{12} + cz_{12} \cos \beta \\ by_{12} \end{pmatrix} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}} \quad (2a) \quad \text{O VIII} \\
\mathbf{B}_{24} &= x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 + \left(z_{12} + \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} ax_{12} + c \left(z_{12} + \frac{1}{2}\right) \cos \beta \\ c \left(z_{12} + \frac{1}{2}\right) \sin \beta \end{pmatrix} \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + \quad (2a) \quad \text{O VIII} \\
\mathbf{B}_{25} &= x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3 = \begin{pmatrix} ax_{13} + cz_{13} \cos \beta \\ by_{13} \end{pmatrix} \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}} \quad (2a) \quad \text{O IX} \\
\mathbf{B}_{26} &= x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 + \left(z_{13} + \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} ax_{13} + c \left(z_{13} + \frac{1}{2}\right) \cos \beta \\ c \left(z_{13} + \frac{1}{2}\right) \sin \beta \end{pmatrix} \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + \quad (2a) \quad \text{O IX} \\
\mathbf{B}_{27} &= x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3 = \begin{pmatrix} ax_{14} + cz_{14} \cos \beta \\ by_{14} \end{pmatrix} \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}} \quad (2a) \quad \text{O X} \\
\mathbf{B}_{28} &= x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 + \left(z_{14} + \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} ax_{14} + c \left(z_{14} + \frac{1}{2}\right) \cos \beta \\ c \left(z_{14} + \frac{1}{2}\right) \sin \beta \end{pmatrix} \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + \quad (2a) \quad \text{O X} \\
\mathbf{B}_{29} &= x_{15} \mathbf{a}_1 + y_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3 = \begin{pmatrix} ax_{15} + cz_{15} \cos \beta \\ by_{15} \end{pmatrix} \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \sin \beta \hat{\mathbf{z}} \quad (2a) \quad \text{O XI} \\
\mathbf{B}_{30} &= x_{15} \mathbf{a}_1 - y_{15} \mathbf{a}_2 + \left(z_{15} + \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} ax_{15} + c \left(z_{15} + \frac{1}{2}\right) \cos \beta \\ c \left(z_{15} + \frac{1}{2}\right) \sin \beta \end{pmatrix} \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} + \quad (2a) \quad \text{O XI} \\
\mathbf{B}_{31} &= x_{16} \mathbf{a}_1 + y_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3 = \begin{pmatrix} ax_{16} + cz_{16} \cos \beta \\ by_{16} \end{pmatrix} \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} + cz_{16} \sin \beta \hat{\mathbf{z}} \quad (2a) \quad \text{O XII} \\
\mathbf{B}_{32} &= x_{16} \mathbf{a}_1 - y_{16} \mathbf{a}_2 + \left(z_{16} + \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} ax_{16} + c \left(z_{16} + \frac{1}{2}\right) \cos \beta \\ c \left(z_{16} + \frac{1}{2}\right) \sin \beta \end{pmatrix} \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} + \quad (2a) \quad \text{O XII} \\
\mathbf{B}_{33} &= x_{17} \mathbf{a}_1 + y_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3 = \begin{pmatrix} ax_{17} + cz_{17} \cos \beta \\ by_{17} \end{pmatrix} \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} + cz_{17} \sin \beta \hat{\mathbf{z}} \quad (2a) \quad \text{Ti I} \\
\mathbf{B}_{34} &= x_{17} \mathbf{a}_1 - y_{17} \mathbf{a}_2 + \left(z_{17} + \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} ax_{17} + c \left(z_{17} + \frac{1}{2}\right) \cos \beta \\ c \left(z_{17} + \frac{1}{2}\right) \sin \beta \end{pmatrix} \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} + \quad (2a) \quad \text{Ti I} \\
\mathbf{B}_{35} &= x_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3 = \begin{pmatrix} ax_{18} + cz_{18} \cos \beta \\ by_{18} \end{pmatrix} \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} + cz_{18} \sin \beta \hat{\mathbf{z}} \quad (2a) \quad \text{Ti II} \\
\mathbf{B}_{36} &= x_{18} \mathbf{a}_1 - y_{18} \mathbf{a}_2 + \left(z_{18} + \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} ax_{18} + c \left(z_{18} + \frac{1}{2}\right) \cos \beta \\ c \left(z_{18} + \frac{1}{2}\right) \sin \beta \end{pmatrix} \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} + \quad (2a) \quad \text{Ti II} \\
\mathbf{B}_{37} &= x_{19} \mathbf{a}_1 + y_{19} \mathbf{a}_2 + z_{19} \mathbf{a}_3 = \begin{pmatrix} ax_{19} + cz_{19} \cos \beta \\ by_{19} \end{pmatrix} \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} + cz_{19} \sin \beta \hat{\mathbf{z}} \quad (2a) \quad \text{Ti III} \\
\mathbf{B}_{38} &= x_{19} \mathbf{a}_1 - y_{19} \mathbf{a}_2 + \left(z_{19} + \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} ax_{19} + c \left(z_{19} + \frac{1}{2}\right) \cos \beta \\ c \left(z_{19} + \frac{1}{2}\right) \sin \beta \end{pmatrix} \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} + \quad (2a) \quad \text{Ti III}
\end{aligned}$$

References

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