Monoclinic $Bi_4Ti_3O_{12}$ $m = 3$ Aurivillius Structure: A4B12C3_mP38_7_4a_12a_3a-001

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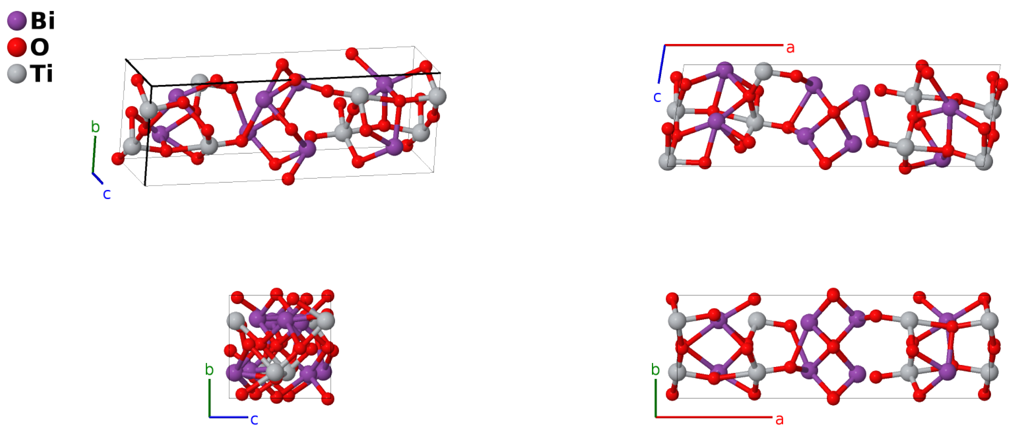
https://aflow.org/p/S41T

https://aflow.org/p/A4B12C3_mP38_7_4a_12a_3a-001



Prototype	$Bi_4O_{12}Ti_3$
AFLOW prototype label	A4B12C3_mP38_7_4a_12a_3a-001
ICSD	38993
Pearson symbol	mP38
Space group number	7
Space group symbol	Pc
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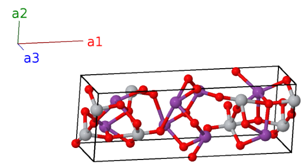
- Aurivillius phases are layered tetragonal materials with composition $(\mathrm{Me}'_2\mathrm{O}_2)^{2+}(\mathrm{Me}_{m-1}\mathrm{R}_m\mathrm{O}_{3m+1})^{2-}$ $(\mathrm{Me}_{m-1}\mathrm{Me}'_2\mathrm{R}_m\mathrm{O}_{3(m+1)})$, where Me and Me' are metals and R is a transition metal with a charge of +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 0.5Å in the atomic positions this structure becomes virtually identical with the orthorhombic structure found by (Dorrian, 1971).

Simple Monoclinic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



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
$\mathbf{B_2}$	=	$x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_1 + c\left(z_1 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(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
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(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
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(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
$\mathbf{B_8}$	=	$x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{10}}$	=	$x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{12}}$	=	$x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_6 + c\left(z_6 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{14}}$	=	$x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_7 + c\left(z_7 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{16}}$	=	$x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_8 + c\left(z_8 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{18}}$	=	$x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_9 + c\left(z_9 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{20}}$	=	$x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{10} + c\left(z_{10} + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(2a)	O VI
$\mathbf{B_{21}}$	=	$x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(2a)	O VII
$\mathbf{B_{22}}$	=	$x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{11} + c\left(z_{11} + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(2a)	O VII
$\mathbf{B_{23}}$	=	$x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(2a)	O VIII

$\mathbf{B_{24}}$	=	$x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 + \left(z_{12}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{12} + c\left(z_{12}+\frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_{12}\,\mathbf{\hat{y}} + c\left(z_{12}+\frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(2a)	O VIII
$\mathbf{B_{25}}$	=	$x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$\left(ax_{13} + cz_{13}\cos\beta\right)\,\mathbf{\hat{x}} + by_{13}\,\mathbf{\hat{y}} + cz_{13}\sin\beta\,\mathbf{\hat{z}}$	(2a)	O IX
$\mathbf{B_{26}}$	=	$x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 + \left(z_{13}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{13} + c\left(z_{13}+\frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_{13}\,\mathbf{\hat{y}} + c\left(z_{13}+\frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(2a)	O IX
$\mathbf{B_{27}}$	=	$x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3$	=	$\left(ax_{14} + cz_{14}\cos\beta\right)\,\mathbf{\hat{x}} + by_{14}\,\mathbf{\hat{y}} + cz_{14}\sin\beta\,\mathbf{\hat{z}}$	(2a)	O X
$\mathbf{B_{28}}$	=	$x_{14}\,\mathbf{a}_1 - y_{14}\,\mathbf{a}_2 + \left(z_{14}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{14} + c\left(z_{14}+\frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_{14}\,\mathbf{\hat{y}} + c\left(z_{14}+\frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(2a)	O X
$\mathbf{B_{29}}$	=	$x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3$	=	$\left(ax_{15} + cz_{15}\cos\beta\right)\,\mathbf{\hat{x}} + by_{15}\,\mathbf{\hat{y}} + cz_{15}\sin\beta\,\mathbf{\hat{z}}$	(2a)	O XI
$\mathbf{B_{30}}$	=	$x_{15}\,\mathbf{a}_1 - y_{15}\,\mathbf{a}_2 + \left(z_{15}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{15} + c\left(z_{15}+\frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_{15}\,\mathbf{\hat{y}} + c\left(z_{15}+\frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(2a)	O XI
$\mathbf{B_{31}}$	=	$x_{16}\,\mathbf{a}_1 + y_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3$	=	$\left(ax_{16} + cz_{16}\cos\beta\right)\,\mathbf{\hat{x}} + by_{16}\,\mathbf{\hat{y}} + cz_{16}\sin\beta\,\mathbf{\hat{z}}$	(2a)	O XII
$\mathbf{B_{32}}$	=	$x_{16}\,\mathbf{a}_1 - y_{16}\,\mathbf{a}_2 + \left(z_{16}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{16} + c\left(z_{16}+\frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_{16}\,\mathbf{\hat{y}} + c\left(z_{16}+\frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(2a)	O XII
$\mathbf{B_{33}}$	=	$x_{17}\,\mathbf{a}_1 + y_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3$	=	$\left(ax_{17} + cz_{17}\cos\beta\right)\,\mathbf{\hat{x}} + by_{17}\,\mathbf{\hat{y}} + cz_{17}\sin\beta\,\mathbf{\hat{z}}$	(2a)	Ti I
$\mathbf{B_{34}}$	=	$x_{17}\,\mathbf{a}_1 - y_{17}\,\mathbf{a}_2 + \left(z_{17}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{17} + c\left(z_{17}+\frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_{17}\,\mathbf{\hat{y}} + c\left(z_{17}+\frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(2a)	Ti I
$\mathbf{B_{35}}$	=	$x_{18}\,\mathbf{a}_1 + y_{18}\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3$	=	$\left(ax_{18} + cz_{18}\cos\beta\right)\,\mathbf{\hat{x}} + by_{18}\,\mathbf{\hat{y}} + cz_{18}\sin\beta\,\mathbf{\hat{z}}$	(2a)	Ti II
$\mathbf{B_{36}}$	=	$x_{18}\,\mathbf{a}_1 - y_{18}\,\mathbf{a}_2 + \left(z_{18}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{18} + c\left(z_{18}+\frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_{18}\,\mathbf{\hat{y}} + c\left(z_{18}+\frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(2a)	Ti II
$\mathbf{B_{37}}$	=	$x_{19}\,\mathbf{a}_1 + y_{19}\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3$	=	$\left(ax_{19} + cz_{19}\cos\beta\right)\,\mathbf{\hat{x}} + by_{19}\,\mathbf{\hat{y}} + cz_{19}\sin\beta\,\mathbf{\hat{z}}$	(2a)	Ti III
$\mathbf{B_{38}}$	=	$x_{19}\,\mathbf{a}_1 - y_{19}\,\mathbf{a}_2 + \left(z_{19}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{19} + c\left(z_{19}+\frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_{19}\,\mathbf{\hat{y}} + c\left(z_{19}+\frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(2a)	Ti III

References

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