Orthorhombic $Bi_4Ti_3O_{12}$ $m = 3$ Aurivillius Structure (*Obsolete*): A4B12C3_oC76_41_2b_6b_ab-001

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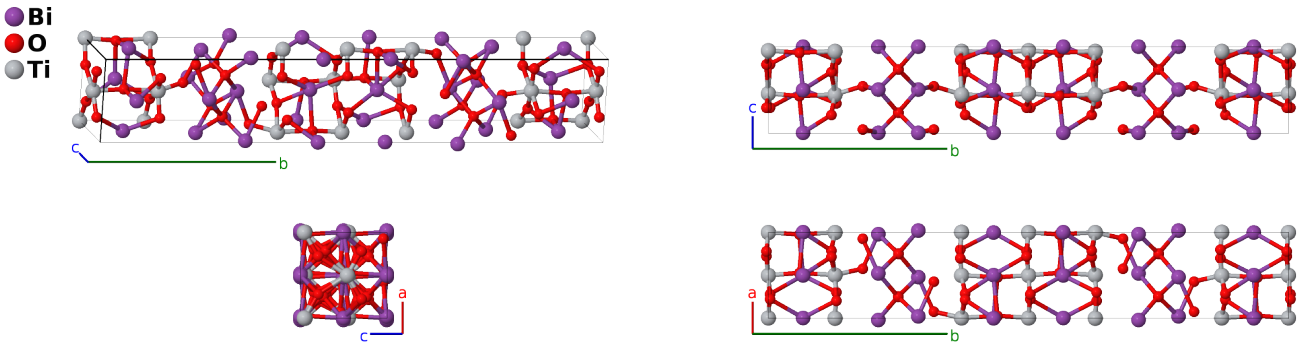
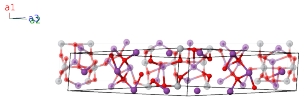


Prototype	$Bi_4O_{12}Ti_3$
AFLOW prototype label	A4B12C3_oC76_41_2b_6b_ab-001
ICSD	16488
Pearson symbol	oC76
Space group number	41
Space group symbol	$Aea2$
AFLOW prototype command	`aflow --proto=A4B12C3_oC76_41_2b_6b_ab-001 --params=`$a, b/a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}$

- Aurivillius phases are layered tetragonal materials with composition $(Me'_2O_2)^{2+}(Me_{m-1}R_mO_{3m+1})^{2-}$ $(Me_{m-1}Me'_2R_mO_{3(m+1)})$, where Me and Me' are metals and R is a transition metal with a charge of +4 or +5. (Subbaro, 1962)
- (Dorrian, 1971) give this structure in what they call the $B2cb$ (or $B2ab$) setting of space group #41. We used FINDSYM to transform this to the standard $Aba2$ setting.
- (Dorrian, 1971) notes that the physical properties of this structure indicate monoclinic symmetry, but that the structure is consistent with orthorhombic symmetry. Various authors have shown that the structure is actually in monoclinic, with space group Pc #7, as described by (Guo, 2019).

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-z_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(4a)	Ti I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	Ti I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + (y_2 - z_2)\,\mathbf{a}_2 + (y_2 + z_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8b)	Bi I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - (y_2 + z_2)\,\mathbf{a}_2 - (y_2 - z_2)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8b)	Bi I
$\mathbf{B_5}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 + z_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_2 + z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8b)	Bi I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 - z_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_2 + z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8b)	Bi I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + (y_3 - z_3)\,\mathbf{a}_2 + (y_3 + z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8b)	Bi II
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 - (y_3 + z_3)\,\mathbf{a}_2 - (y_3 - z_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8b)	Bi II
$\mathbf{B_9}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8b)	Bi II
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8b)	Bi II
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1 + (y_4 - z_4)\,\mathbf{a}_2 + (y_4 + z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{12}}$	=	$-x_4\,\mathbf{a}_1 - (y_4 + z_4)\,\mathbf{a}_2 - (y_4 - z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{13}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 - z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{15}}$	=	$x_5\,\mathbf{a}_1 + (y_5 - z_5)\,\mathbf{a}_2 + (y_5 + z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_{16}}$	=	$-x_5\,\mathbf{a}_1 - (y_5 + z_5)\,\mathbf{a}_2 - (y_5 - z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_{17}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_{18}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5 - z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_{19}}$	=	$x_6\,\mathbf{a}_1 + (y_6 - z_6)\,\mathbf{a}_2 + (y_6 + z_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_{20}}$	=	$-x_6\,\mathbf{a}_1 - (y_6 + z_6)\,\mathbf{a}_2 - (y_6 - z_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_{21}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6 + z_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_{22}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6 - z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_{23}}$	=	$x_7\,\mathbf{a}_1 + (y_7 - z_7)\,\mathbf{a}_2 + (y_7 + z_7)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8b)	O IV
$\mathbf{B_{24}}$	=	$-x_7\,\mathbf{a}_1 - (y_7 + z_7)\,\mathbf{a}_2 - (y_7 - z_7)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8b)	O IV

$\mathbf{B_{25}}$	=	$\left(x_7+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_7+z_7-\frac{1}{2}\right)\,\mathbf{a}_2+\left(-y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(8b)	O IV
$\mathbf{B_{26}}$	=	$-\left(x_7-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_7-z_7+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_7+z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_7+\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(8b)	O IV
$\mathbf{B_{27}}$	=	$x_8\,\mathbf{a}_1+(y_8-z_8)\,\mathbf{a}_2+(y_8+z_8)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8b)	O V
$\mathbf{B_{28}}$	=	$-x_8\,\mathbf{a}_1-(y_8+z_8)\,\mathbf{a}_2-(y_8-z_8)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8b)	O V
$\mathbf{B_{29}}$	=	$\left(x_8+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_8+z_8-\frac{1}{2}\right)\,\mathbf{a}_2+\left(-y_8+z_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_8+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_8-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8b)	O V
$\mathbf{B_{30}}$	=	$-\left(x_8-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_8-z_8+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_8+z_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_8-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_8+\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8b)	O V
$\mathbf{B_{31}}$	=	$x_9\,\mathbf{a}_1+(y_9-z_9)\,\mathbf{a}_2+(y_9+z_9)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(8b)	O VI
$\mathbf{B_{32}}$	=	$-x_9\,\mathbf{a}_1-(y_9+z_9)\,\mathbf{a}_2-(y_9-z_9)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(8b)	O VI
$\mathbf{B_{33}}$	=	$\left(x_9+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_9+z_9-\frac{1}{2}\right)\,\mathbf{a}_2+\left(-y_9+z_9+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_9+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_9-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(8b)	O VI
$\mathbf{B_{34}}$	=	$-\left(x_9-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_9-z_9+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_9+z_9+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_9-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_9+\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(8b)	O VI
$\mathbf{B_{35}}$	=	$x_{10}\,\mathbf{a}_1+(y_{10}-z_{10})\,\mathbf{a}_2+(y_{10}+z_{10})\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(8b)	Ti II
$\mathbf{B_{36}}$	=	$-x_{10}\,\mathbf{a}_1-(y_{10}+z_{10})\,\mathbf{a}_2-(y_{10}-z_{10})\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(8b)	Ti II
$\mathbf{B_{37}}$	=	$\left(x_{10}+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_{10}+z_{10}-\frac{1}{2}\right)\,\mathbf{a}_2+\left(-y_{10}+z_{10}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_{10}+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_{10}-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(8b)	Ti II
$\mathbf{B_{38}}$	=	$-\left(x_{10}-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_{10}-z_{10}+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_{10}+z_{10}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_{10}-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_{10}+\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}}$	(8b)	Ti II

References

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