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

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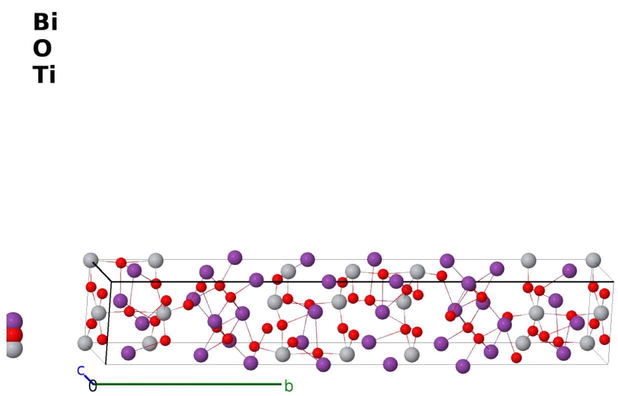
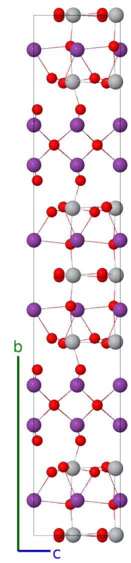
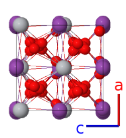
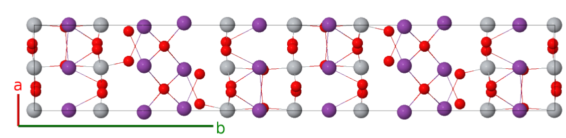
https://aflow.org/prototype-encyclopedia/A4B12C3_oC76_41_2b_6b_ab-001









Prototype $Bi_4O_{12}Ti_3$

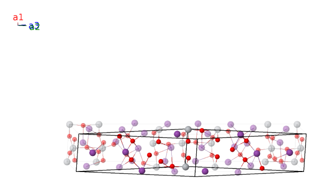
AFLOW prototype label A4B12C3_oC76_41_2b_6b_ab-001

ICSD	16488
CCDC	1597063
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 $(\mathrm{Me}'_2\mathrm{O}_2)^{2+}(\mathrm{Me}_{m-1}\mathrm{R}_m\mathrm{O}_{3m+1})^{2-}$ $(\mathrm{Me}_{m-1}\mathrm{Me}'_2\mathrm{R}_m\mathrm{O}_{3(m+1)})$, where Me and Me' are metals and R is a transition metal with a charge of +4 or +5. (Subbaro, 1962)
- (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

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



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

$\mathbf{B_{8}}$	=	$-x_{3}\,\mathbf{a}_{1} - \left(y_{3}+z_{3}\right)\,\mathbf{a}_{2} - \left(y_{3}-z_{3}\right)\,\mathbf{a}_{3}$	=	$-ax_{3}\,\hat{\mathbf{x}} - by_{3}\,\hat{\mathbf{y}} + cz_{3}\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{11}}$	=	$x_{4}\,\mathbf{a}_{1} + \left(y_{4}-z_{4}\right)\,\mathbf{a}_{2} + \left(y_{4}+z_{4}\right)\,\mathbf{a}_{3}$	=	$ax_{4}\,\hat{\mathbf{x}} + by_{4}\,\hat{\mathbf{y}} + cz_{4}\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{12}}$	=	$-x_{4}\,\mathbf{a}_{1} - \left(y_{4}+z_{4}\right)\,\mathbf{a}_{2} - \left(y_{4}-z_{4}\right)\,\mathbf{a}_{3}$	=	$-ax_{4}\,\hat{\mathbf{x}} - by_{4}\,\hat{\mathbf{y}} + cz_{4}\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{15}}$	=	$x_{5}\,\mathbf{a}_{1} + \left(y_{5}-z_{5}\right)\,\mathbf{a}_{2} + \left(y_{5}+z_{5}\right)\,\mathbf{a}_{3}$	=	$ax_{5}\,\hat{\mathbf{x}} + by_{5}\,\hat{\mathbf{y}} + cz_{5}\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_{16}}$	=	$-x_{5}\,\mathbf{a}_{1} - \left(y_{5}+z_{5}\right)\,\mathbf{a}_{2} - \left(y_{5}-z_{5}\right)\,\mathbf{a}_{3}$	=	$-ax_{5}\,\hat{\mathbf{x}} - by_{5}\,\hat{\mathbf{y}} + cz_{5}\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{19}}$	=	$x_{6}\,\mathbf{a}_{1} + \left(y_{6}-z_{6}\right)\,\mathbf{a}_{2} + \left(y_{6}+z_{6}\right)\,\mathbf{a}_{3}$	=	$ax_{6}\,\hat{\mathbf{x}} + by_{6}\,\hat{\mathbf{y}} + cz_{6}\,\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_{20}}$	=	$-x_{6}\,\mathbf{a}_{1} - \left(y_{6}+z_{6}\right)\,\mathbf{a}_{2} - \left(y_{6}-z_{6}\right)\,\mathbf{a}_{3}$	=	$-ax_{6}\,\hat{\mathbf{x}} - by_{6}\,\hat{\mathbf{y}} + cz_{6}\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{23}}$	=	$x_{7}\,\mathbf{a}_{1} + \left(y_{7}-z_{7}\right)\,\mathbf{a}_{2} + \left(y_{7}+z_{7}\right)\,\mathbf{a}_{3}$	=	$ax_{7}\,\hat{\mathbf{x}} + by_{7}\,\hat{\mathbf{y}} + cz_{7}\,\hat{\mathbf{z}}$	(8b)	O IV
$\mathbf{B_{24}}$	=	$-x_{7}\,\mathbf{a}_{1} - \left(y_{7}+z_{7}\right)\,\mathbf{a}_{2} - \left(y_{7}-z_{7}\right)\,\mathbf{a}_{3}$	=	$-ax_{7}\,\hat{\mathbf{x}} - by_{7}\,\hat{\mathbf{y}} + cz_{7}\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{27}}$	=	$x_{8}\,\mathbf{a}_{1} + \left(y_{8}-z_{8}\right)\,\mathbf{a}_{2} + \left(y_{8}+z_{8}\right)\,\mathbf{a}_{3}$	=	$ax_{8}\,\hat{\mathbf{x}} + by_{8}\,\hat{\mathbf{y}} + cz_{8}\,\hat{\mathbf{z}}$	(8b)	O V
$\mathbf{B_{28}}$	=	$-x_{8}\,\mathbf{a}_{1} - \left(y_{8}+z_{8}\right)\,\mathbf{a}_{2} - \left(y_{8}-z_{8}\right)\,\mathbf{a}_{3}$	=	$-ax_{8}\,\hat{\mathbf{x}} - by_{8}\,\hat{\mathbf{y}} + cz_{8}\,\hat{\mathbf{z}}$	(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

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