

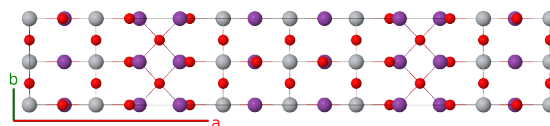
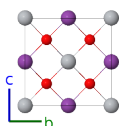
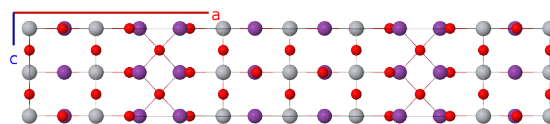
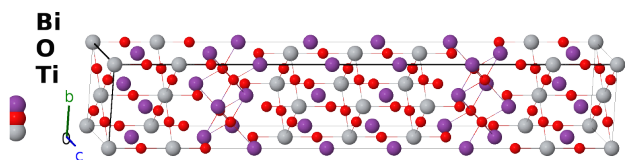
Orthorhombic Bi₄Ti₃O₁₂ $m = 3$ Aurivillius Structure: A4B12C3_oF76_69_2g_cf2gl_ag-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, 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/Y2ES>

https://aflow.org/prototype-encyclopedia/A4B12C3_oF76_69_2g_cf2gl_ag-001



Prototype	Bi ₄ O ₁₂ Ti ₃
AFLOW prototype label	A4B12C3_oF76_69_2g_cf2gl_ag-001
ICSD	24735
CCDC	1600747
Pearson symbol	oF76
Space group number	69
Space group symbol	<i>Fmmm</i>
AFLOW prototype command	<code>aflow --proto=A4B12C3_oF76_69_2g_cf2gl_ag-001</code> <code>--params=a, b/a, c/a, x₄, x₅, x₆, x₇, x₈, x₉</code>

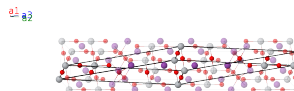
- Aurivillius phases are layered tetragonal materials with composition (Me'₂O₂)²⁺(Me_{m-1}R_mO_{3m+1})²⁻(Me_{m-1}Me'₂R_mO_{3(m+1)}), where Me and Me' are metals and R is a transition metal with a charge of +4 or +5. (Subbaro, 1962)
- This is the original structural determination by (Aurivillius, 1949). It should not be confused with the obsolete $m = 3$ Aurivillius structure in space group *Aea2* #41.

Face-centered Orthorhombic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}c\hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(4a) Ti I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8c) O I
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8c) O I
$\mathbf{B}_4$	$=$	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8f) O II
$\mathbf{B}_5$	$=$	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8f) O II
$\mathbf{B}_6$	$=$	$-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}}$	(8g) Bi I
$\mathbf{B}_7$	$=$	$x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}}$	(8g) Bi I
$\mathbf{B}_8$	$=$	$-x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}}$	(8g) Bi II
$\mathbf{B}_9$	$=$	$x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}}$	(8g) Bi II
$\mathbf{B}_{10}$	$=$	$-x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}}$	(8g) O III
$\mathbf{B}_{11}$	$=$	$x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - x_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}}$	(8g) O III
$\mathbf{B}_{12}$	$=$	$-x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}}$	(8g) O IV
$\mathbf{B}_{13}$	$=$	$x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}}$	(8g) O IV
$\mathbf{B}_{14}$	$=$	$-x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}}$	(8g) Ti II
$\mathbf{B}_{15}$	$=$	$x_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - x_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}}$	(8g) Ti II
$\mathbf{B}_{16}$	$=$	$-(x_9 - \frac{1}{2}) \mathbf{a}_1 + x_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(16l) O V
$\mathbf{B}_{17}$	$=$	$x_9 \mathbf{a}_1 - (x_9 - \frac{1}{2}) \mathbf{a}_2 - (x_9 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(16l) O V
$\mathbf{B}_{18}$	$=$	$(x_9 + \frac{1}{2}) \mathbf{a}_1 - x_9 \mathbf{a}_2 - x_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(16l) O V
$\mathbf{B}_{19}$	$=$	$-x_9 \mathbf{a}_1 + (x_9 + \frac{1}{2}) \mathbf{a}_2 + (x_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(16l) O V

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First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.