# Orthorhombic $Bi_4Ti_3O_{12}$ $m = 3$ Aurivillius Structure: A4B12C3_oF76_69_2g_cf2gl_ag-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

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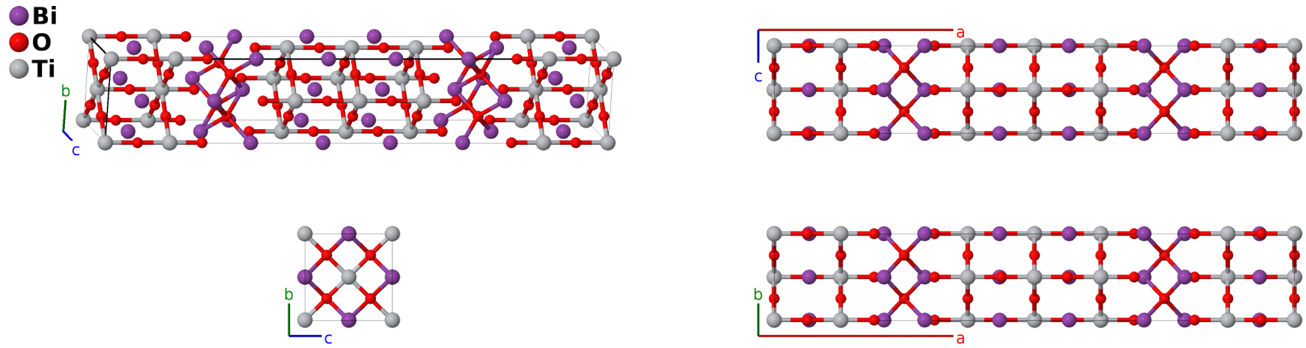
https://aflow.org/p/A4B12C3_oF76_69_2g_cf2gl_ag-001




| | |
|---|---|
| **Prototype** | $Bi_4O_{12}Ti_3$ |
| **AFLOW prototype label** | A4B12C3_oF76_69_2g_cf2gl_ag-001 |
| **ICSD** | 24735 |
| **Pearson symbol** | oF76 |
| **Space group number** | 69 |
| **Space group symbol** | $Fmmm$ |
| **AFLOW prototype command** | `aflow --proto=A4B12C3_oF76_69_2g_cf2gl_ag-001 --params=`$a, b/a, c/a, x_4, x_5, x_6, x_7, x_8, x_9$ |

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- 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)
- 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.

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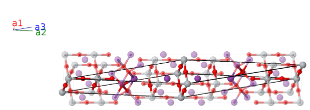
### Face-centered Orthorhombic primitive vectors

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



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### 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 |
| $\mathbf{B_{16}}$ | = | $-\left(x_9-\frac{1}{2}\right)\,\mathbf{a}_1+x_9\,\mathbf{a}_2+x_9\,\mathbf{a}_3$ | = | $ax_9\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$ | (16l) | O V |
| $\mathbf{B_{17}}$ | = | $x_9\,\mathbf{a}_1-\left(x_9-\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_9-\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(x_9-\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$ | (16l) | O V |
| $\mathbf{B_{18}}$ | = | $\left(x_9+\frac{1}{2}\right)\,\mathbf{a}_1-x_9\,\mathbf{a}_2-x_9\,\mathbf{a}_3$ | = | $-ax_9\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$ | (16l) | O V |
| $\mathbf{B_{19}}$ | = | $-x_9\,\mathbf{a}_1+\left(x_9+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_9+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $a\left(x_9+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$ | (16l) | O V |

## References


[1] B. Aurivillius, *Mixed bismuth oxides with layer lattices II. Structure of $Bi_4Ti_3O_{12}$*, Arkiv för Kemi **1**, 499–512 (1949).

[2] E. C. Subbarao, *A family of ferroelectric bismuth compounds*, J. Phys.: Conf. Ser. **23**, 665–676 (1962), doi:10.1016/0022-3697(62)90526-7.

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[4] J. F. Dorrian, R. E. Newnham, D. K. Smith, and M. I. Kay, *Crystal Structure of $Bi_4Ti_3O_{12}$*, Ferroelectrics **3**, 17–27 (1972), doi:10.1080/00150197108237680.