

Bi₇(Fe,Ti)₆O₂₁ $m = 6$ Aurivillius Structure: A7B6C21_oF136_42_a3c_3c_ab3c3e-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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/M0MD>

https://aflow.org/prototype-encyclopedia/A7B6C21_oF136_42_a3c_3c_ab3c3e-001

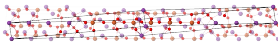
Prototype	Bi ₇ Fe ₃ O ₂₁
AFLOW prototype label	A7B6C21_oF136_42_a3c_3c_ab3c3e-001
ICSD	155931
CCDC	1672502
Pearson symbol	oF136
Space group number	42
Space group symbol	$Fmm2$
AFLOW prototype command	<pre>aflow --proto=A7B6C21_oF136_42_a3c_3c_ab3c3e-001 --params=a,b/a,c/a,z₁,z₂,z₃,y₄,z₄,y₅,z₅,y₆,z₆,y₇,z₇,y₈,z₈,y₉,z₉,y₁₀,z₁₀,y₁₁,z₁₁, y₁₂,z₁₂,x₁₃,y₁₃,z₁₃,x₁₄,y₁₄,z₁₄,x₁₅,y₁₅,z₁₅</pre>

- Aurivillius phases are layered tetragonal materials with composition $(\text{Me}'_2\text{O}_2)^{2+}(\text{Me}_{m-1}\text{R}_m\text{O}_{3m+1})^{2-}$ $(\text{Me}_{m-1}\text{Me}'_2\text{R}_m\text{O}_{3(m+1)})$, where Me and Me' are metals and R is a transition metal with a charge of +4 or +5. (Subbaro, 1962).
- The iron and titanium atoms are randomly distributed across the transition metal (8c) sites. We have arbitrarily labeled them as iron.
- (Krzyszhanovskaya, 2005) gave the structure in the $F2mm$ setting of space group #42. We swapped the y - and z -axes to transform this to the standard $Fmm2$ setting.

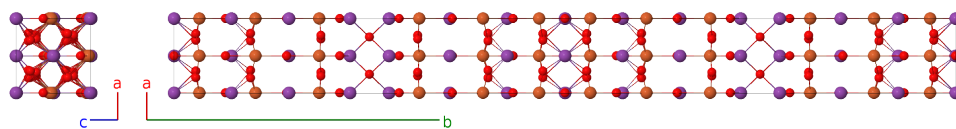
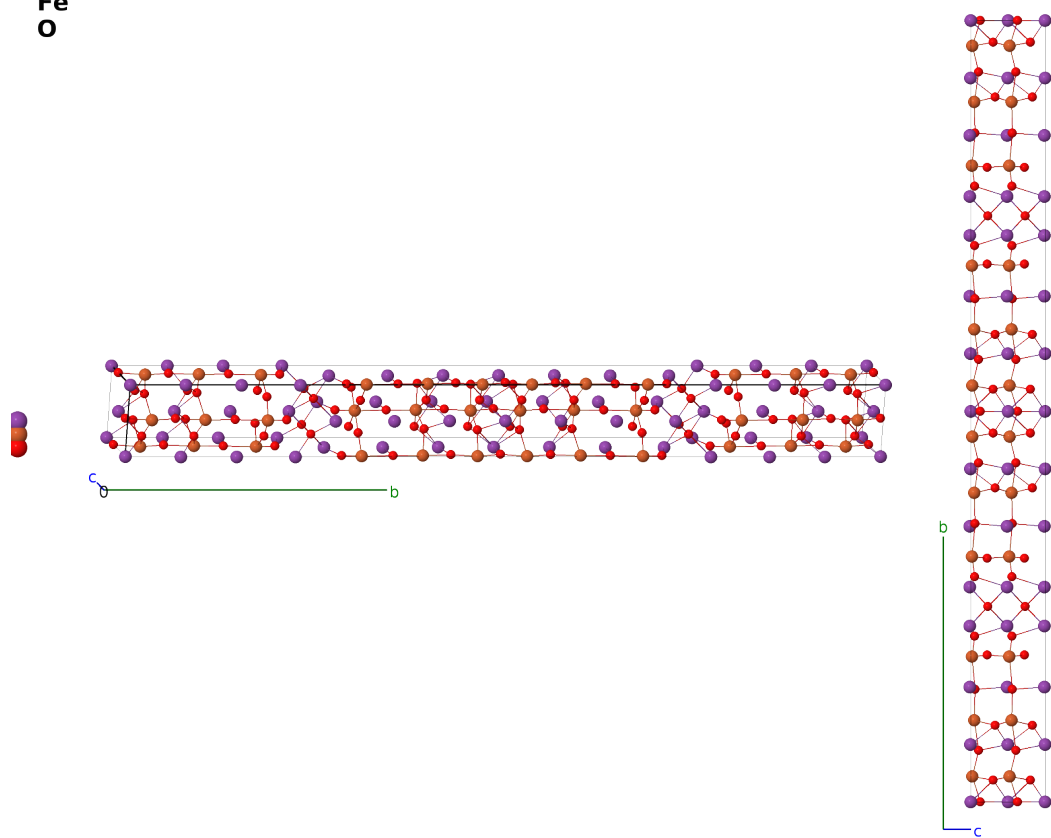
Face-centered Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} \end{aligned}$$





Bi
Fe
O



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(4a)	Bi I
$\mathbf{B}_2$	$= z_2 \mathbf{a}_1 + z_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_3$	$= z_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B}_4$	$= (z_3 + \frac{1}{2}) \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B}_5$	$= (y_4 + z_4) \mathbf{a}_1 - (y_4 - z_4) \mathbf{a}_2 + (y_4 - z_4) \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8c)	Bi II
$\mathbf{B}_6$	$= -(y_4 - z_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 - (y_4 + z_4) \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8c)	Bi II
$\mathbf{B}_7$	$= (y_5 + z_5) \mathbf{a}_1 - (y_5 - z_5) \mathbf{a}_2 + (y_5 - z_5) \mathbf{a}_3$	$=$	$by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8c)	Bi III
$\mathbf{B}_8$	$= -(y_5 - z_5) \mathbf{a}_1 + (y_5 + z_5) \mathbf{a}_2 - (y_5 + z_5) \mathbf{a}_3$	$=$	$-by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8c)	Bi III
$\mathbf{B}_9$	$= (y_6 + z_6) \mathbf{a}_1 - (y_6 - z_6) \mathbf{a}_2 + (y_6 - z_6) \mathbf{a}_3$	$=$	$by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8c)	Bi IV
$\mathbf{B}_{10}$	$= -(y_6 - z_6) \mathbf{a}_1 + (y_6 + z_6) \mathbf{a}_2 - (y_6 + z_6) \mathbf{a}_3$	$=$	$-by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8c)	Bi IV
$\mathbf{B}_{11}$	$= (y_7 + z_7) \mathbf{a}_1 - (y_7 - z_7) \mathbf{a}_2 + (y_7 - z_7) \mathbf{a}_3$	$=$	$by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B}_{12}$	$= -(y_7 - z_7) \mathbf{a}_1 + (y_7 + z_7) \mathbf{a}_2 - (y_7 + z_7) \mathbf{a}_3$	$=$	$-by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B}_{13}$	$= (y_8 + z_8) \mathbf{a}_1 - (y_8 - z_8) \mathbf{a}_2 + (y_8 - z_8) \mathbf{a}_3$	$=$	$by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8c)	Fe II
$\mathbf{B}_{14}$	$= -(y_8 - z_8) \mathbf{a}_1 + (y_8 + z_8) \mathbf{a}_2 - (y_8 + z_8) \mathbf{a}_3$	$=$	$-by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8c)	Fe II
$\mathbf{B}_{15}$	$= (y_9 + z_9) \mathbf{a}_1 - (y_9 - z_9) \mathbf{a}_2 + (y_9 - z_9) \mathbf{a}_3$	$=$	$by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8c)	Fe III
$\mathbf{B}_{16}$	$= -(y_9 - z_9) \mathbf{a}_1 + (y_9 + z_9) \mathbf{a}_2 - (y_9 + z_9) \mathbf{a}_3$	$=$	$-by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8c)	Fe III
$\mathbf{B}_{17}$	$= (y_{10} + z_{10}) \mathbf{a}_1 - (y_{10} - z_{10}) \mathbf{a}_2 + (y_{10} - z_{10}) \mathbf{a}_3$	$=$	$by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B}_{18}$	$= -(y_{10} - z_{10}) \mathbf{a}_1 + (y_{10} + z_{10}) \mathbf{a}_2 - (y_{10} + z_{10}) \mathbf{a}_3$	$=$	$-by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B}_{19}$	$= (y_{11} + z_{11}) \mathbf{a}_1 - (y_{11} - z_{11}) \mathbf{a}_2 + (y_{11} - z_{11}) \mathbf{a}_3$	$=$	$by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(8c)	O IV
$\mathbf{B}_{20}$	$= -(y_{11} - z_{11}) \mathbf{a}_1 + (y_{11} + z_{11}) \mathbf{a}_2 - (y_{11} + z_{11}) \mathbf{a}_3$	$=$	$-by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(8c)	O IV
$\mathbf{B}_{21}$	$= (y_{12} + z_{12}) \mathbf{a}_1 - (y_{12} - z_{12}) \mathbf{a}_2 + (y_{12} - z_{12}) \mathbf{a}_3$	$=$	$by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$	(8c)	O V
$\mathbf{B}_{22}$	$= -(y_{12} - z_{12}) \mathbf{a}_1 + (y_{12} + z_{12}) \mathbf{a}_2 - (y_{12} + z_{12}) \mathbf{a}_3$	$=$	$-by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$	(8c)	O V
$\mathbf{B}_{23}$	$= (-x_{13} + y_{13} + z_{13}) \mathbf{a}_1 + (x_{13} - y_{13} + z_{13}) \mathbf{a}_2 + (x_{13} + y_{13} - z_{13}) \mathbf{a}_3$	$=$	$ax_{13} \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}}$	(16e)	O VI

$$\begin{aligned}
\mathbf{B}_{24} &= \begin{pmatrix} (x_{13} - y_{13} + z_{13}) \mathbf{a}_1 + \\ (-x_{13} + y_{13} + z_{13}) \mathbf{a}_2 - \\ (x_{13} + y_{13} + z_{13}) \mathbf{a}_3 \end{pmatrix} = -ax_{13} \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (16e) & \text{O VI} \\
\mathbf{B}_{25} &= \begin{pmatrix} -(x_{13} + y_{13} - z_{13}) \mathbf{a}_1 + \\ (x_{13} + y_{13} + z_{13}) \mathbf{a}_2 + \\ (x_{13} - y_{13} - z_{13}) \mathbf{a}_3 \end{pmatrix} = ax_{13} \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (16e) & \text{O VI} \\
\mathbf{B}_{26} &= \begin{pmatrix} (x_{13} + y_{13} + z_{13}) \mathbf{a}_1 - \\ (x_{13} + y_{13} - z_{13}) \mathbf{a}_2 - \\ (x_{13} - y_{13} + z_{13}) \mathbf{a}_3 \end{pmatrix} = -ax_{13} \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (16e) & \text{O VI} \\
\mathbf{B}_{27} &= \begin{pmatrix} (-x_{14} + y_{14} + z_{14}) \mathbf{a}_1 + \\ (x_{14} - y_{14} + z_{14}) \mathbf{a}_2 + \\ (x_{14} + y_{14} - z_{14}) \mathbf{a}_3 \end{pmatrix} = ax_{14} \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (16e) & \text{O VII} \\
\mathbf{B}_{28} &= \begin{pmatrix} (x_{14} - y_{14} + z_{14}) \mathbf{a}_1 + \\ (-x_{14} + y_{14} + z_{14}) \mathbf{a}_2 - \\ (x_{14} + y_{14} + z_{14}) \mathbf{a}_3 \end{pmatrix} = -ax_{14} \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (16e) & \text{O VII} \\
\mathbf{B}_{29} &= \begin{pmatrix} -(x_{14} + y_{14} - z_{14}) \mathbf{a}_1 + \\ (x_{14} + y_{14} + z_{14}) \mathbf{a}_2 + \\ (x_{14} - y_{14} - z_{14}) \mathbf{a}_3 \end{pmatrix} = ax_{14} \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (16e) & \text{O VII} \\
\mathbf{B}_{30} &= \begin{pmatrix} (x_{14} + y_{14} + z_{14}) \mathbf{a}_1 - \\ (x_{14} + y_{14} - z_{14}) \mathbf{a}_2 - \\ (x_{14} - y_{14} + z_{14}) \mathbf{a}_3 \end{pmatrix} = -ax_{14} \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (16e) & \text{O VII} \\
\mathbf{B}_{31} &= \begin{pmatrix} (-x_{15} + y_{15} + z_{15}) \mathbf{a}_1 + \\ (x_{15} - y_{15} + z_{15}) \mathbf{a}_2 + \\ (x_{15} + y_{15} - z_{15}) \mathbf{a}_3 \end{pmatrix} = ax_{15} \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (16e) & \text{O VIII} \\
\mathbf{B}_{32} &= \begin{pmatrix} (x_{15} - y_{15} + z_{15}) \mathbf{a}_1 + \\ (-x_{15} + y_{15} + z_{15}) \mathbf{a}_2 - \\ (x_{15} + y_{15} + z_{15}) \mathbf{a}_3 \end{pmatrix} = -ax_{15} \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (16e) & \text{O VIII} \\
\mathbf{B}_{33} &= \begin{pmatrix} -(x_{15} + y_{15} - z_{15}) \mathbf{a}_1 + \\ (x_{15} + y_{15} + z_{15}) \mathbf{a}_2 + \\ (x_{15} - y_{15} - z_{15}) \mathbf{a}_3 \end{pmatrix} = ax_{15} \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (16e) & \text{O VIII} \\
\mathbf{B}_{34} &= \begin{pmatrix} (x_{15} + y_{15} + z_{15}) \mathbf{a}_1 - \\ (x_{15} + y_{15} - z_{15}) \mathbf{a}_2 - \\ (x_{15} - y_{15} + z_{15}) \mathbf{a}_3 \end{pmatrix} = -ax_{15} \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (16e) & \text{O VIII}
\end{aligned}$$

References

- [1] M. Krzhizhanovskaya, S. Filatov, V. Gusarov, P. Paufler, R. Bubnova, M. Morozov, and D. C. Meyer, *Aurivillius Phases in the $\text{Bi}_4\text{Ti}_3\text{O}_{12}/\text{BiFeO}_3$ System: Thermal Behaviour and Crystal Structure*, *Z. Anorganische und Allgemeine Chemie* **631**, 1603–1608 (2005), doi:10.1002/zaac.200500130.
- [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.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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.