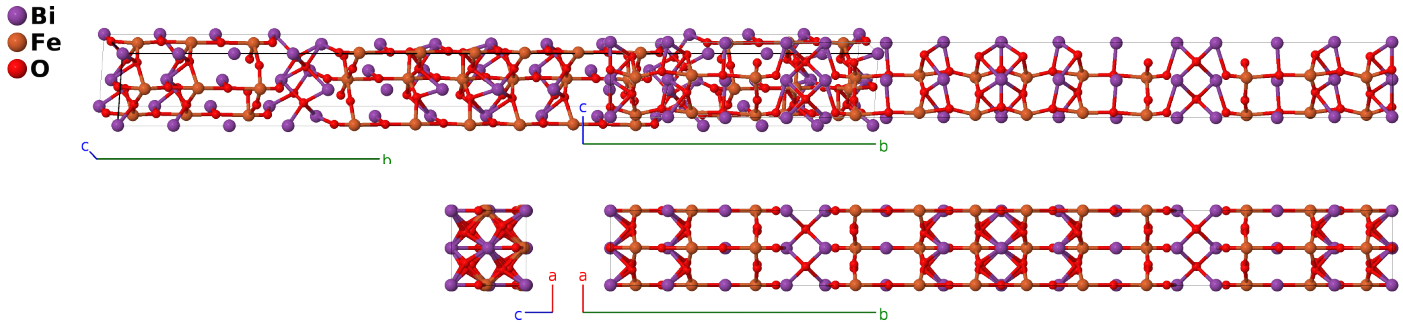


Bi₇(Fe,Ti)₆O₂₁ $m = 6$ Aurivillius Structure: A7B6C21_oF136_42_a3c_3c_ab3c3e-001

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<https://aflow.org/p/M0MD>

https://aflow.org/p/A7B6C21_oF136_42_a3c_3c_ab3c3e-001

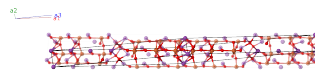


Prototype	Bi ₇ Fe ₃ O ₂₁
AFLOW prototype label	A7B6C21_oF136_42_a3c_3c_ab3c3e-001
ICSD	155931
Pearson symbol	oF136
Space group number	42
Space group symbol	<i>Fmm2</i>
AFLOW prototype command	aflow --proto=A7B6C21_oF136_42_a3c_3c_ab3c3e-001 --params= $a, b/a, c/a, z_1, z_2, z_3, y_4, z_4, y_5, z_5, y_6, z_6, y_7, z_7, y_8, z_8, y_9, z_9, y_{10}, z_{10}, y_{11}, z_{11}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}$

- 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.
- (Krzhizhanovskaya, 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

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



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
\mathbf{B}_{24}	$= (x_{13} - y_{13} + z_{13}) \mathbf{a}_1 +$ $(-x_{13} + y_{13} + z_{13}) \mathbf{a}_2 -$ $(x_{13} + y_{13} + z_{13}) \mathbf{a}_3$	$=$	$-ax_{13} \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}}$	(16e)	O VI

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

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