$LaTi_3Bi_4$ Structure: A4BC3_oF64_69_gho_g_gl-001

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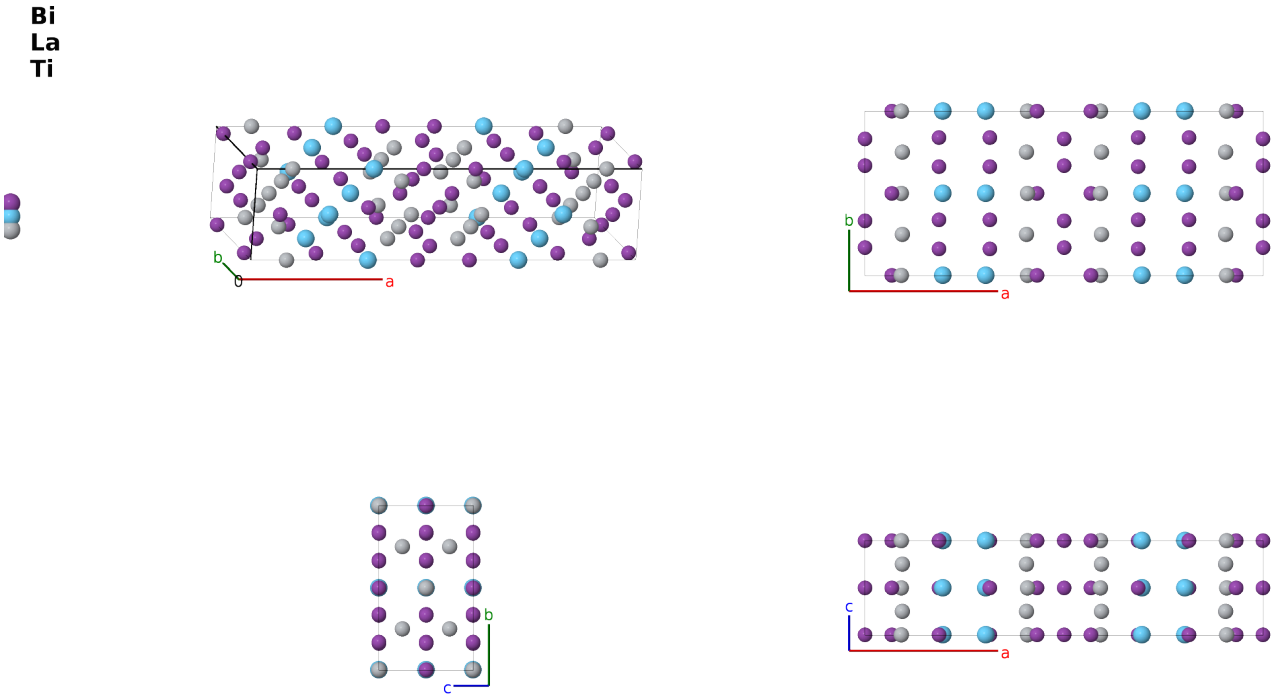
https://aflow.org/prototype-encyclopedia/TN6Q

https://aflow.org/prototype-encyclopedia/A4BC3_oF64_69_gho_g_gl-001



Prototype	Bi_4LaTi_3
AFLOW prototype label	A4BC3_oF64_69_gho_g_gl-001
ICSD	119550
CCDC	2335975
Pearson symbol	oF64
Space group number	69
Space group symbol	$Fmmm$
AFLOW prototype command	`aflow --proto=A4BC3_oF64_69_gho_g_gl-001 --params=`$a, b/a, c/a, x_1, x_2, x_3, y_4, x_5, x_6, y_6$

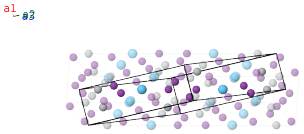
Other compounds with this structure

$CaTi_3Bi_4$, CaV_3Sb_4, $CeTi_3Bi_4$, $DyTi_3Bi_4$, $ErTi_3Bi_4$, $EuTi_3Bi_4$, $GdTi_3Bi_4$, $HoTi_3Bi_4$, $LuTi_3Bi_4$, $NdTi_3Bi_4$, $PmTi_3Bi_4$, $PrTi_3Bi_4$, $SmTi_3Bi_4$, $TbTi_3Bi_4$, $TmTi_3Bi_4$, $YbTi_3Bi_4$, $Nd(Sb, Sn)_3Bi_4$

- In orthorhombic systems the AFLOW prototype label standard favors orientations of where most of the free atomic parameters are along the x-axis. Thus we have rotated the published structure so that coordinates (x,y,z) → (z,y,-x), with a similar change for the lattice parameters.
- The ICSD lists $Nd(Sb,Sn)_3Bi_4$ as the prototype for this structure, but we prefer to use a fully ordered structure.

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
$\mathbf{B_1}$	=	$-x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}}$	(8g)	Bi I
$\mathbf{B_2}$	=	$x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}}$	(8g)	Bi I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}$	(8g)	La I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}$	(8g)	La I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(8g)	Ti I
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(8g)	Ti I
$\mathbf{B_7}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}}$	(8h)	Bi II
$\mathbf{B_8}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}}$	(8h)	Bi II
$\mathbf{B_9}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16l)	Ti II
$\mathbf{B_{10}}$	=	$x_5\,\mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16l)	Ti II
$\mathbf{B_{11}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16l)	Ti II
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16l)	Ti II
$\mathbf{B_{13}}$	=	$-\left(x_6 - y_6\right)\,\mathbf{a}_1 + \left(x_6 - y_6\right)\,\mathbf{a}_2 + \left(x_6 + y_6\right)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}}$	(16o)	Bi III
$\mathbf{B_{14}}$	=	$\left(x_6 - y_6\right)\,\mathbf{a}_1 - \left(x_6 - y_6\right)\,\mathbf{a}_2 - \left(x_6 + y_6\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}}$	(16o)	Bi III
$\mathbf{B_{15}}$	=	$\left(x_6 + y_6\right)\,\mathbf{a}_1 - \left(x_6 + y_6\right)\,\mathbf{a}_2 - \left(x_6 - y_6\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}}$	(16o)	Bi III
$\mathbf{B_{16}}$	=	$-\left(x_6 + y_6\right)\,\mathbf{a}_1 + \left(x_6 + y_6\right)\,\mathbf{a}_2 + \left(x_6 - y_6\right)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}}$	(16o)	Bi III

References

[1] B. R. Ortiz, H. Miao, D. S. Parker, F. Yang, G. D. Samolyuk, E. M. Clements, A. Rajapitamahuni, T. Yilmaz, E. Vescovo, J. Yan, A. F. May, and M. A. McGuire, *Evolution of Highly Anisotropic Magnetism in the Titanium-Based Kagome Metals $LnTi_3Bi_4$ (Ln: La···Gd^{3+}, Eu^{2+}, Yb^{2+})*, Chem. of Mater. **35**, 9756–9773 (2023), doi:10.1021/acs.chemmater.3c02289.

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