Orthorhombic Bi_3NbTiO_9 $m = 2$ Aurivillius Structure: A3B2C9_oF56_69_ag_g_bfgl-001

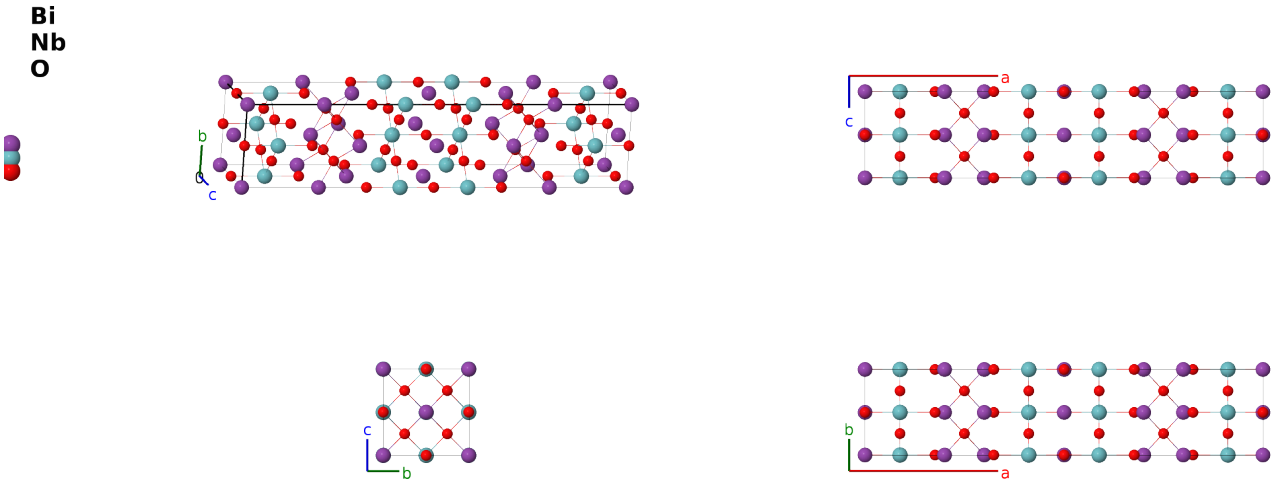
Cite this page as:

- 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/FSA1

https://aflow.org/prototype-encyclopedia/A3B2C9_oF56_69_ag_g_bfgl-001



Prototype	$Bi_3Nb_2O_9$
AFLOW prototype label	A3B2C9_oF56_69_ag_g_bfgl-001
ICSD	24734
CCDC	1600746
Pearson symbol	oF56
Space group number	69
Space group symbol	$Fmmm$
AFLOW prototype command	`aflow --proto=A3B2C9_oF56_69_ag_g_bfgl-001 --params=`$a, b/a, c/a, x_4, x_5, x_6, x_7$

Other compounds with this structure

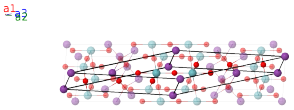
$BaBi_2Nb_2O_9$, $CaBi_2Nb_2O_9$, $KBi_2Nb_2O_9$, $NaBi_2Nb_2O_9$, $PbBi_2Nb_2O_9$, $SrBi_2Nb_2O_9$

- 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). The niobium and titanium atoms equally occupy the same (8g) site. We have arbitrarily labeled this as "Nb."

- Crystals such as $BaBi_2Nb_2O_9$ put the non-bismuth atom on the (4a) site, and the niobium site can be occupied by niobium, tantalum, and/or titanium. (Aurivillius, 1949)
- We have swapped Aurivillius's x- and z-axes.

Face-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Bi I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4b)	O I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_5}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}$	(8g)	Bi 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 II
$\mathbf{B_7}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}$	(8g)	Nb 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)	Nb I
$\mathbf{B_9}$	=	$-x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}}$	(8g)	O III
$\mathbf{B_{10}}$	=	$x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}}$	(8g)	O III
$\mathbf{B_{11}}$	=	$-\left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16l)	O IV
$\mathbf{B_{12}}$	=	$x_7\,\mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16l)	O IV
$\mathbf{B_{13}}$	=	$\left(x_7 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16l)	O IV
$\mathbf{B_{14}}$	=	$-x_7\,\mathbf{a}_1 + \left(x_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_7 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16l)	O IV

References

[1] B. Aurivillius, *Mixed bismuth oxides with layer lattices I. The structure type $CaNb_2Bi_2O_9$*, Arkiv för Kemi **1**, 463–479 (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.

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.