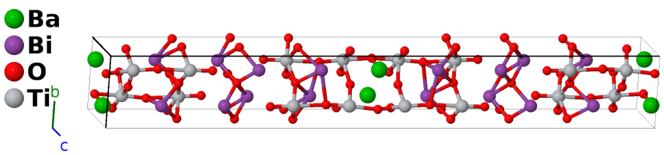
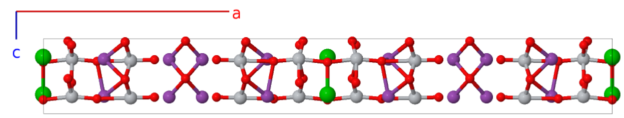
Low Temperature $BaBi_4Ti_4O_{15}$ Structure: AB4C15D4_oC96_36_a_2b_a7b_2b-001

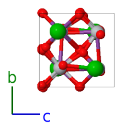
Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

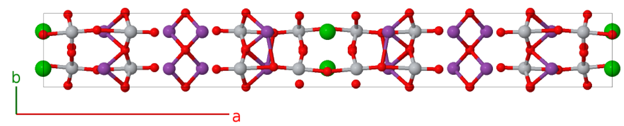
https://aflow.org/p/8N75

https://aflow.org/p/AB4C15D4_oC96_36_a_2b_a7b_2b-001







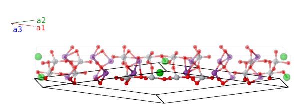


Prototype	$BaBi_4O_{15}Ti_4$
AFLOW prototype label	AB4C15D4_oC96_36_a_2b_a7b_2b-001
ICSD	150928
Pearson symbol	oC96
Space group number	36
Space group symbol	$Cmc2_1$
AFLOW prototype command	`aflow --proto=AB4C15D4_oC96_36_a_2b_a7b_2b-001` `--params=`$a, b/a, c/a, y_1, z_1, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}$

- 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)
- Data for this structure was taken at room temperature. Above 700K this transforms into the tetragonal high temperature $m = 4$ Aurivillius structure.
- The ICSD entry for this structure states that the actual composition of what we call the Ba I site is $Ba_{0.26}Bi_{0.74}$, and the composition of our Bi II site is $Ba_{0.37}Bi_{0.74}$. We have arbitrarily labeled the first of these sites Ba and the second Bi so that the AFLOW label mimics the composition of the structure.
- (Kennedy, 2003) give the structural information in the $A2_1am$ setting of space group # 36. We used FINDSYM to transform this to the standard $Cmc2_1$ setting.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	Ba I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ba I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_5}$	=	$(x_3 - y_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8b)	Bi I
$\mathbf{B_6}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - (x_3 + y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	Bi I
$\mathbf{B_7}$	=	$(x_3 + y_3)\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	Bi I
$\mathbf{B_8}$	=	$-(x_3 + y_3)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8b)	Bi I
$\mathbf{B_9}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8b)	Bi II
$\mathbf{B_{10}}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	Bi II
$\mathbf{B_{11}}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	Bi II
$\mathbf{B_{12}}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8b)	Bi II
$\mathbf{B_{13}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_{14}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - (x_5 + y_5)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_{15}}$	=	$(x_5 + y_5)\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_{16}}$	=	$-(x_5 + y_5)\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_{17}}$	=	$(x_6 - y_6)\,\mathbf{a}_1 + (x_6 + y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_{18}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - (x_6 + y_6)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_{19}}$	=	$(x_6 + y_6)\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_{20}}$	=	$-(x_6 + y_6)\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_{21}}$	=	$(x_7 - y_7)\,\mathbf{a}_1 + (x_7 + y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8b)	O IV
$\mathbf{B_{22}}$	=	$-(x_7 - y_7)\,\mathbf{a}_1 - (x_7 + y_7)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	O IV
$\mathbf{B_{23}}$	=	$(x_7 + y_7)\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	O IV
$\mathbf{B_{24}}$	=	$-(x_7 + y_7)\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8b)	O IV

$\mathbf{B_{25}}$	=	$\left(x_{8}-y_{8}\right)\,\mathbf{a}_{1}+\left(x_{8}+y_{8}\right)\,\mathbf{a}_{2}+z_{8}\,\mathbf{a}_{3}$	=	$ax_{8}\,\mathbf{\hat{x}}+by_{8}\,\mathbf{\hat{y}}+cz_{8}\,\mathbf{\hat{z}}$	(8b)	O V
$\mathbf{B_{26}}$	=	$-\left(x_{8}-y_{8}\right)\,\mathbf{a}_{1}-\left(x_{8}+y_{8}\right)\,\mathbf{a}_{2}+\left(z_{8}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-ax_{8}\,\mathbf{\hat{x}}-by_{8}\,\mathbf{\hat{y}}+c\left(z_{8}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O V
$\mathbf{B_{27}}$	=	$\left(x_{8}+y_{8}\right)\,\mathbf{a}_{1}+\left(x_{8}-y_{8}\right)\,\mathbf{a}_{2}+\left(z_{8}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$ax_{8}\,\mathbf{\hat{x}}-by_{8}\,\mathbf{\hat{y}}+c\left(z_{8}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O V
$\mathbf{B_{28}}$	=	$-\left(x_{8}+y_{8}\right)\,\mathbf{a}_{1}-\left(x_{8}-y_{8}\right)\,\mathbf{a}_{2}+z_{8}\,\mathbf{a}_{3}$	=	$-ax_{8}\,\mathbf{\hat{x}}+by_{8}\,\mathbf{\hat{y}}+cz_{8}\,\mathbf{\hat{z}}$	(8b)	O V
$\mathbf{B_{29}}$	=	$\left(x_{9}-y_{9}\right)\,\mathbf{a}_{1}+\left(x_{9}+y_{9}\right)\,\mathbf{a}_{2}+z_{9}\,\mathbf{a}_{3}$	=	$ax_{9}\,\mathbf{\hat{x}}+by_{9}\,\mathbf{\hat{y}}+cz_{9}\,\mathbf{\hat{z}}$	(8b)	O VI
$\mathbf{B_{30}}$	=	$-\left(x_{9}-y_{9}\right)\,\mathbf{a}_{1}-\left(x_{9}+y_{9}\right)\,\mathbf{a}_{2}+\left(z_{9}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-ax_{9}\,\mathbf{\hat{x}}-by_{9}\,\mathbf{\hat{y}}+c\left(z_{9}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O VI
$\mathbf{B_{31}}$	=	$\left(x_{9}+y_{9}\right)\,\mathbf{a}_{1}+\left(x_{9}-y_{9}\right)\,\mathbf{a}_{2}+\left(z_{9}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$ax_{9}\,\mathbf{\hat{x}}-by_{9}\,\mathbf{\hat{y}}+c\left(z_{9}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O VI
$\mathbf{B_{32}}$	=	$-\left(x_{9}+y_{9}\right)\,\mathbf{a}_{1}-\left(x_{9}-y_{9}\right)\,\mathbf{a}_{2}+z_{9}\,\mathbf{a}_{3}$	=	$-ax_{9}\,\mathbf{\hat{x}}+by_{9}\,\mathbf{\hat{y}}+cz_{9}\,\mathbf{\hat{z}}$	(8b)	O VI
$\mathbf{B_{33}}$	=	$\left(x_{10}-y_{10}\right)\,\mathbf{a}_{1}+\left(x_{10}+y_{10}\right)\,\mathbf{a}_{2}+z_{10}\,\mathbf{a}_{3}$	=	$ax_{10}\,\mathbf{\hat{x}}+by_{10}\,\mathbf{\hat{y}}+cz_{10}\,\mathbf{\hat{z}}$	(8b)	O VII
$\mathbf{B_{34}}$	=	$-\left(x_{10}-y_{10}\right)\,\mathbf{a}_{1}-\left(x_{10}+y_{10}\right)\,\mathbf{a}_{2}+\left(z_{10}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-ax_{10}\,\mathbf{\hat{x}}-by_{10}\,\mathbf{\hat{y}}+c\left(z_{10}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O VII
$\mathbf{B_{35}}$	=	$\left(x_{10}+y_{10}\right)\,\mathbf{a}_{1}+\left(x_{10}-y_{10}\right)\,\mathbf{a}_{2}+\left(z_{10}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$ax_{10}\,\mathbf{\hat{x}}-by_{10}\,\mathbf{\hat{y}}+c\left(z_{10}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O VII
$\mathbf{B_{36}}$	=	$-\left(x_{10}+y_{10}\right)\,\mathbf{a}_{1}-\left(x_{10}-y_{10}\right)\,\mathbf{a}_{2}+z_{10}\,\mathbf{a}_{3}$	=	$-ax_{10}\,\mathbf{\hat{x}}+by_{10}\,\mathbf{\hat{y}}+cz_{10}\,\mathbf{\hat{z}}$	(8b)	O VII
$\mathbf{B_{37}}$	=	$\left(x_{11}-y_{11}\right)\,\mathbf{a}_{1}+\left(x_{11}+y_{11}\right)\,\mathbf{a}_{2}+z_{11}\,\mathbf{a}_{3}$	=	$ax_{11}\,\mathbf{\hat{x}}+by_{11}\,\mathbf{\hat{y}}+cz_{11}\,\mathbf{\hat{z}}$	(8b)	O VIII
$\mathbf{B_{38}}$	=	$-\left(x_{11}-y_{11}\right)\,\mathbf{a}_{1}-\left(x_{11}+y_{11}\right)\,\mathbf{a}_{2}+\left(z_{11}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-ax_{11}\,\mathbf{\hat{x}}-by_{11}\,\mathbf{\hat{y}}+c\left(z_{11}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O VIII
$\mathbf{B_{39}}$	=	$\left(x_{11}+y_{11}\right)\,\mathbf{a}_{1}+\left(x_{11}-y_{11}\right)\,\mathbf{a}_{2}+\left(z_{11}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$ax_{11}\,\mathbf{\hat{x}}-by_{11}\,\mathbf{\hat{y}}+c\left(z_{11}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O VIII
$\mathbf{B_{40}}$	=	$-\left(x_{11}+y_{11}\right)\,\mathbf{a}_{1}-\left(x_{11}-y_{11}\right)\,\mathbf{a}_{2}+z_{11}\,\mathbf{a}_{3}$	=	$-ax_{11}\,\mathbf{\hat{x}}+by_{11}\,\mathbf{\hat{y}}+cz_{11}\,\mathbf{\hat{z}}$	(8b)	O VIII
$\mathbf{B_{41}}$	=	$\left(x_{12}-y_{12}\right)\,\mathbf{a}_{1}+\left(x_{12}+y_{12}\right)\,\mathbf{a}_{2}+z_{12}\,\mathbf{a}_{3}$	=	$ax_{12}\,\mathbf{\hat{x}}+by_{12}\,\mathbf{\hat{y}}+cz_{12}\,\mathbf{\hat{z}}$	(8b)	Ti I
$\mathbf{B_{42}}$	=	$-\left(x_{12}-y_{12}\right)\,\mathbf{a}_{1}-\left(x_{12}+y_{12}\right)\,\mathbf{a}_{2}+\left(z_{12}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-ax_{12}\,\mathbf{\hat{x}}-by_{12}\,\mathbf{\hat{y}}+c\left(z_{12}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	Ti I
$\mathbf{B_{43}}$	=	$\left(x_{12}+y_{12}\right)\,\mathbf{a}_{1}+\left(x_{12}-y_{12}\right)\,\mathbf{a}_{2}+\left(z_{12}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$ax_{12}\,\mathbf{\hat{x}}-by_{12}\,\mathbf{\hat{y}}+c\left(z_{12}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	Ti I
$\mathbf{B_{44}}$	=	$-\left(x_{12}+y_{12}\right)\,\mathbf{a}_{1}-\left(x_{12}-y_{12}\right)\,\mathbf{a}_{2}+z_{12}\,\mathbf{a}_{3}$	=	$-ax_{12}\,\mathbf{\hat{x}}+by_{12}\,\mathbf{\hat{y}}+cz_{12}\,\mathbf{\hat{z}}$	(8b)	Ti I
$\mathbf{B_{45}}$	=	$\left(x_{13}-y_{13}\right)\,\mathbf{a}_{1}+\left(x_{13}+y_{13}\right)\,\mathbf{a}_{2}+z_{13}\,\mathbf{a}_{3}$	=	$ax_{13}\,\mathbf{\hat{x}}+by_{13}\,\mathbf{\hat{y}}+cz_{13}\,\mathbf{\hat{z}}$	(8b)	Ti II
$\mathbf{B_{46}}$	=	$-\left(x_{13}-y_{13}\right)\,\mathbf{a}_{1}-\left(x_{13}+y_{13}\right)\,\mathbf{a}_{2}+\left(z_{13}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-ax_{13}\,\mathbf{\hat{x}}-by_{13}\,\mathbf{\hat{y}}+c\left(z_{13}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	Ti II
$\mathbf{B_{47}}$	=	$\left(x_{13}+y_{13}\right)\,\mathbf{a}_{1}+\left(x_{13}-y_{13}\right)\,\mathbf{a}_{2}+\left(z_{13}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$ax_{13}\,\mathbf{\hat{x}}-by_{13}\,\mathbf{\hat{y}}+c\left(z_{13}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	Ti II
$\mathbf{B_{48}}$	=	$-\left(x_{13}+y_{13}\right)\,\mathbf{a}_{1}-\left(x_{13}-y_{13}\right)\,\mathbf{a}_{2}+z_{13}\,\mathbf{a}_{3}$	=	$-ax_{13}\,\mathbf{\hat{x}}+by_{13}\,\mathbf{\hat{y}}+cz_{13}\,\mathbf{\hat{z}}$	(8b)	Ti II

References

[1] B. J. Kennedy, Y. Kubota, B. A. Hunter, I., and K. Kato, *Structural phase transitions in the layered bismuth oxide* $BaBi_4Ti_4O_{15}$, Solid State Commun. **126**, 653–658 (2003), doi:10.1016/S0038-1098(03)00332-6.

[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.