High Temperature $BaBi_4Ti_4O_{15}$ $m = 4$ Aurivillius Structure: AB4C15D4_tI48_139_a_2e_bd2e2g_2e-001

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https://aflow.org/p/Y186

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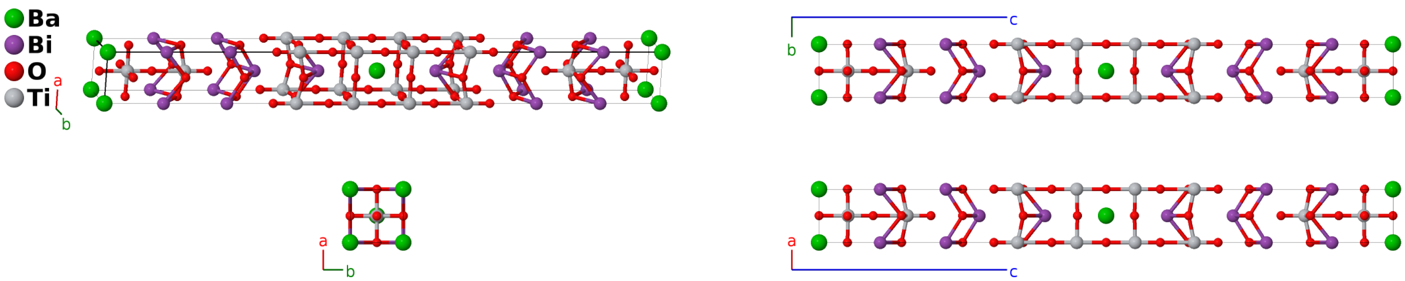


Prototype	$BaBi_4O_{15}Ti_4$
AFLOW prototype label	AB4C15D4_tI48_139_a_2e_bd2e2g_2e-001
ICSD	150929
Pearson symbol	tI48
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=AB4C15D4_tI48_139_a_2e_bd2e2g_2e-001 --params=`$a, c/a, z_4, z_5, z_6, z_7, z_8, z_9, z_{10}, z_{11}$

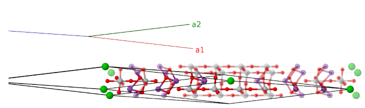
Other compounds with this structure

$PbBi_4Ti_4O_{15}$, $Bi_5Ti_3GaO_{15}$

- 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)
- The ICSD entry for this structure states that the actual composition of our Ba I site is $Ba_{0.26}Bi_{0.74}$, while the Bi II sites composition is $Ba_{0.37}Bi_{0.63}$. 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. The original work of (Aurivillius, 1950) assumes equal mixing of barium and bismuth on all of the Ba/Bi sites.
- Below 700K this structure transforms into the orthorhombic low temperature $BaBi_4Ti_4O_{15}$ structure. (Kennedy, 2003) Data for the illustrated structure was taken at 1000K.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ba I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B_5}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	Bi I
$\mathbf{B_6}$	=	$-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	Bi I
$\mathbf{B_7}$	=	$z_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2$	=	$cz_5\,\hat{\mathbf{z}}$	(4e)	Bi II
$\mathbf{B_8}$	=	$-z_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2$	=	$-cz_5\,\hat{\mathbf{z}}$	(4e)	Bi II
$\mathbf{B_9}$	=	$z_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2$	=	$cz_6\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{10}}$	=	$-z_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2$	=	$-cz_6\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{11}}$	=	$z_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2$	=	$cz_7\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{12}}$	=	$-z_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_2$	=	$-cz_7\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{13}}$	=	$z_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2$	=	$cz_8\,\hat{\mathbf{z}}$	(4e)	Ti I
$\mathbf{B_{14}}$	=	$-z_8\,\mathbf{a}_1 - z_8\,\mathbf{a}_2$	=	$-cz_8\,\hat{\mathbf{z}}$	(4e)	Ti I
$\mathbf{B_{15}}$	=	$z_9\,\mathbf{a}_1 + z_9\,\mathbf{a}_2$	=	$cz_9\,\hat{\mathbf{z}}$	(4e)	Ti II
$\mathbf{B_{16}}$	=	$-z_9\,\mathbf{a}_1 - z_9\,\mathbf{a}_2$	=	$-cz_9\,\hat{\mathbf{z}}$	(4e)	Ti II
$\mathbf{B_{17}}$	=	$\left(z_{10} + \frac{1}{2}\right)\,\mathbf{a}_1 + z_{10}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(8g)	O V
$\mathbf{B_{18}}$	=	$z_{10}\,\mathbf{a}_1 + \left(z_{10} + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_{10}\,\hat{\mathbf{z}}$	(8g)	O V
$\mathbf{B_{19}}$	=	$-\left(z_{10} - \frac{1}{2}\right)\,\mathbf{a}_1 - z_{10}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}}$	(8g)	O V
$\mathbf{B_{20}}$	=	$-z_{10}\,\mathbf{a}_1 - \left(z_{10} - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_{10}\,\hat{\mathbf{z}}$	(8g)	O V
$\mathbf{B_{21}}$	=	$\left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_1 + z_{11}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(8g)	O VI
$\mathbf{B_{22}}$	=	$z_{11}\,\mathbf{a}_1 + \left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_{11}\,\hat{\mathbf{z}}$	(8g)	O VI
$\mathbf{B_{23}}$	=	$-\left(z_{11} - \frac{1}{2}\right)\,\mathbf{a}_1 - z_{11}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}}$	(8g)	O VI
$\mathbf{B_{24}}$	=	$-z_{11}\,\mathbf{a}_1 - \left(z_{11} - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_{11}\,\hat{\mathbf{z}}$	(8g)	O VI

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.

[3] B. Aurivillius, *Mixed oxides with layer lattice. III. Structure of* $BaBi_4Ti_4O_{15}$, Arkiv für Kemi **2**, 519–527 (1950).