Room Temperature Tetragonal $BaTiO_3$ Structure: AB3C_tP5_99_b_ac_a-001

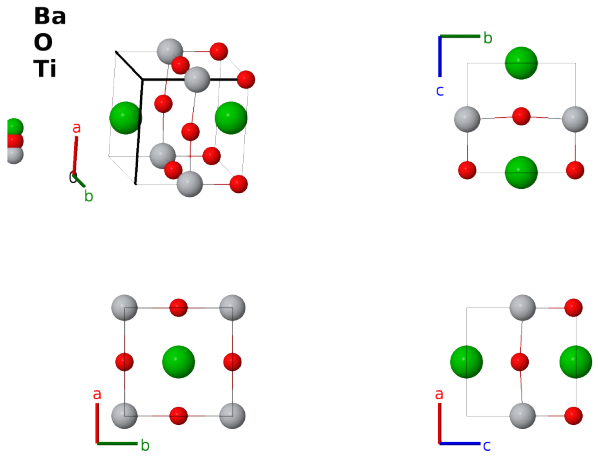
Cite this page as:

- 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/3BZX

https://aflow.org/prototype-encyclopedia/AB3C_tP5_99_b_ac_a-001



Prototype	BaO_3Ti
AFLOW prototype label	AB3C_tP5_99_b_ac_a-001
ICSD	130020
CCDC	1667269
Pearson symbol	tP5
Space group number	99
Space group symbol	$P4mm$
AFLOW prototype command	`aflow --proto=AB3C_tP5_99_b_ac_a-001 --params=`$a, c/a, z_1, z_2, z_3, z_4$

Other compounds with this structure
$CsEuCl_3$, $CsPbBr_3$, $CsPbCl_3$, $CsSrCl_3$, $EuTiO_3$, $GdCoO_3$, $KNbO_3$, $NaNbO_3$, $PbTiO_3$

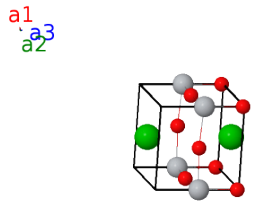
- The perovskite $BaTiO_3$ undergoes a variety of temperature driven phase transitions. (Shirane, 1957)
- The first three structures are ferroelectric:
  - Below 193K the structure is rhombohedral.
  - Between 193K and 278K the structure is orthorhombic.
  - Between 278K and 393K the structure is tetragonal. This room-temperature form of the material is describe here.

  - Above 393K the compound is a cubic perovskite ($E2_1$).

- Hexagonal $BaTiO_3$ can be stabilized by alloying the titanium sites with other transition metals. (Dickson, 1961) The pure structure has been grown at 1853K and cooled to room temperature. (Akimo, 1994)
- This structure has the same space group and occupied Wyckoff positions as the tetragonal PZT structure, but the displacements from the cubic perovskite structure are different, so we give this structure its own AFLOW prototype designation.
- The ICSD lists many compounds under the PZT/"PerovskitePbTiO3(disordered)" structure type. Most of these have considerable alloying on the metallic sites. We collect all the completely ordered structures here.
- Presumably the data for this structure was taken at room temperature.
- Space group *P4mm* #99 does not specify the origin of the z-axis. We set it by taking $z_3 = 0$, putting the barium atom at the origin.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(1a)	O I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(1a)	Ti I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(1b)	Ba I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(2c)	O II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2c)	O II

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.