

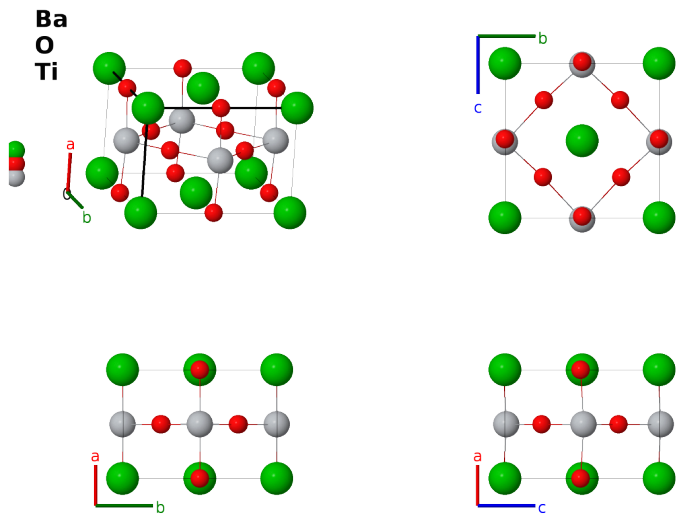
Orthorhombic BaTiO₃ Structure: AB3C_oC10_38_a_ae_b-002

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, 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/8STH>

https://aflow.org/prototype-encyclopedia/AB3C_oC10_38_a_ae_b-002



Prototype	BaO ₃ Ti
AFLOW prototype label	AB3C_oC10_38_a_ae_b-002
ICSD	31155
CCDC	1605312
Pearson symbol	oC10
Space group number	38
Space group symbol	<i>Amm</i> 2
AFLOW prototype command	<code>aflow --proto=AB3C_oC10_38_a_ae_b-002 --params=a, b/a, c/a, z₁, z₂, z₃, y₄, z₄</code>

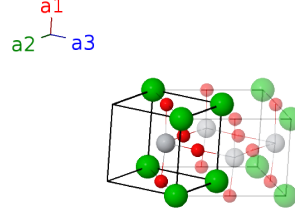
- The perovskite BaTiO₃ undergoes a variety of temperature driven phase transitions. (Shirane, 1957)
- The first three structures are ferroelectric:
 - Below 193K the structure is rhombohedral.
 - Between 193K and 278K the structure is orthorhombic. (This structure)
 - Between 278K and 393K the structure is tetragonal. This is the room-temperature form of the material.

– 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)
- The data for this structure was taken 263K.
- Space group $Amm2$ #38 does not specify the origin of the z -axis. We set it by taking $z_1 = 0$, putting the barium atom at the origin.

Base-centered Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= \frac{1}{2}b \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -z_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(2a)	Ba I
$\mathbf{B}_2$	$= -z_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 - z_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + cz_3 \hat{\mathbf{z}}$	(2b)	Ti I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 + (y_4 + z_4) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 - (y_4 - z_4) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4e)	O II

References

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Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, 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.