Orthorhombic $BaTiO_3$ Structure: AB3C_oC10_38_a_ae_b-002

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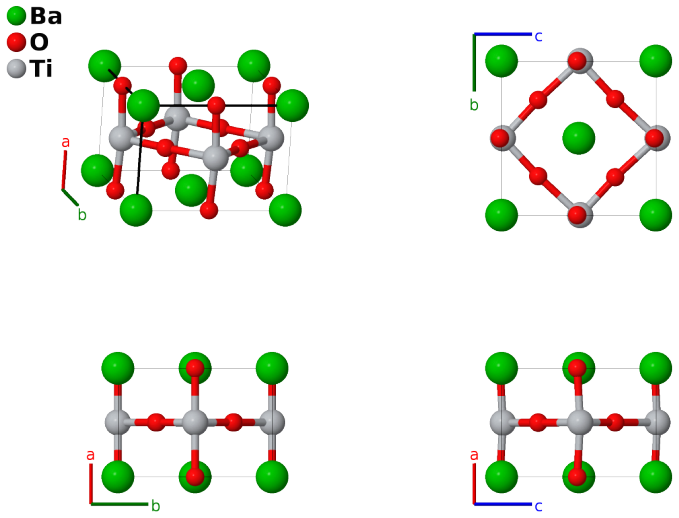
https://aflow.org/p/8STH

https://aflow.org/p/AB3C_oC10_38_a_ae_b-002



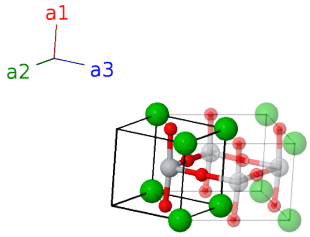
Prototype	BaO_3Ti
AFLOW prototype label	AB3C_oC10_38_a_ae_b-002
ICSD	31155
Pearson symbol	oC10
Space group number	38
Space group symbol	$Amm2$
AFLOW prototype command	`aflow --proto=AB3C_oC10_38_a_ae_b-002 --params=`$a, b/a, c/a, z_1, z_2, z_3, y_4, z_4$

- 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. (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

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



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

[1] G. Shirane, H. Danner, and R. Pepinsky, *Neutron Diffraction Study of Orthorhombic $BaTiO_3$*, Phys. Rev. **105**, 856–860 (1957), doi:10.1103/PhysRev.105.856.

[2] J. G. Dickson, L. Katz, and R. Ward, *Compounds with the Hexagonal Barium Titanate Structure*, J. Am. Chem. Soc. **83**, 3026–3029 (1961), doi:10.1021/ja01475a012.

[3] A. W. Hewat, *Structure of rhombohedral ferroelectric barium titanate*, Ferroelectrics **6**, 215–218 (1974), doi:10.1080/00150197408243970.

[4] J. Akimoto, Y. Gotoh, and Y. Oosawa, *Refinement of Hexagonal $BaTiO_3$*, Acta Crystallogr. Sect. C **50**, 160–161 (1994), doi:10.1107/S0108270193008637.

Found in

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