Rhombohedral $BaTiO_3$ Structure: AB3C_hR5_160_a_b_a-001

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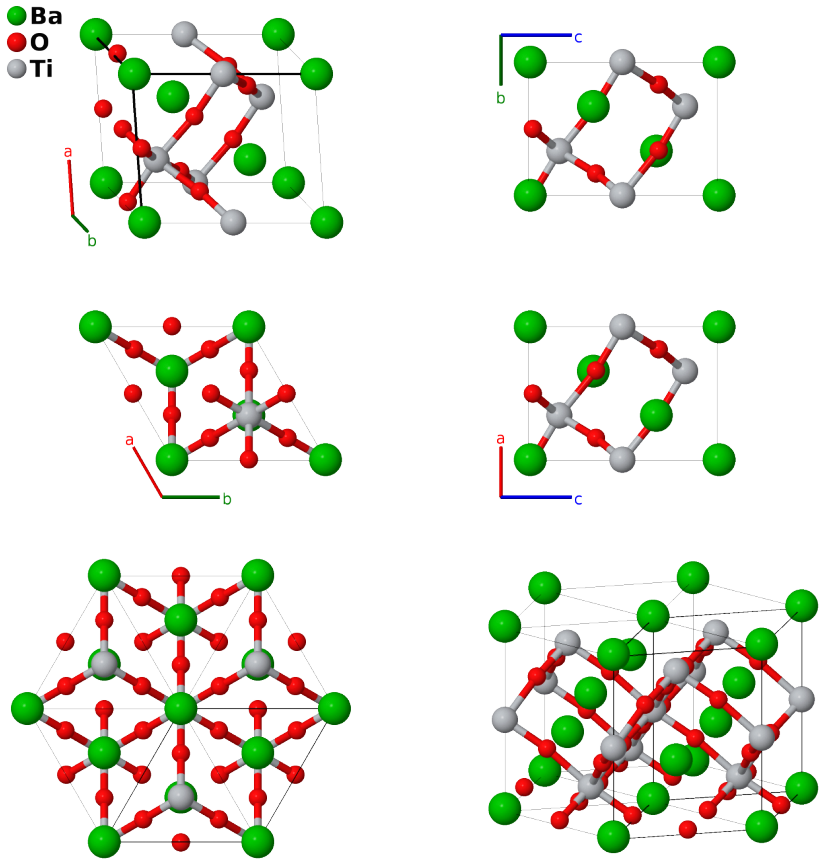
https://aflow.org/p/X85U

https://aflow.org/p/AB3C_hR5_160_a_b_a-001



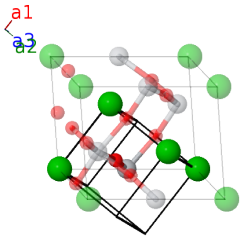
Prototype	BaO_3Ti
AFLOW prototype label	AB3C_hR5_160_a_b_a-001
ICSD	6102
Pearson symbol	hR5
Space group number	160
Space group symbol	$R3m$
AFLOW prototype command	`aflow --proto=AB3C_hR5_160_a_b_a-001 --params=`$a, c/a, x_1, x_2, x_3, z_3$

- 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. (This structure)
  - Between 193K and 278K the structure is orthorhombic.
  - 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 was taken at 77.4K.
- Rhombohedral $BaTiO_3$ is isostructural with γ-KNO_3 and $KBrO_3$ ($G0_7$), but the structural parameters are sufficiently different to warrant adding another structure to the database.
- Space group $R3m$ #160 does not specify the origin of the z-axis. We follow (Hewat, 1974) and place the origin so that the titanium atom is at $1/2c\hat{z}$.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(1a)	Ba I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(1a)	Ti I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(3b)	O I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(3b)	O I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(3b)	O I

References

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