Tetragonal PZT [$Pb(Zr_xTi_{1-x})O_3$] Structure: A3BC_tP5_99_ac_b_a-002

This structure previously used the label(s) `A3BC_tP5_99_bc_a_b`. Calls to these addresses will be redirected here.

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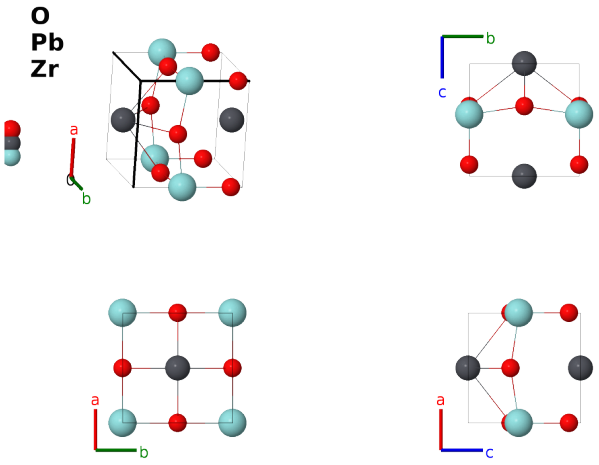
https://aflow.org/prototype-encyclopedia/Z2SB

https://aflow.org/prototype-encyclopedia/A3BC_tP5_99_ac_b_a-002



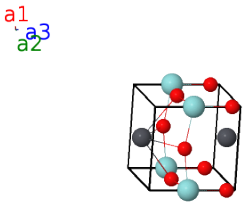
Prototype	O_3PbZr
AFLOW prototype label	A3BC_tP5_99_ac_b_a-002
Mineral name	'PZT'
ICSD	92059
CCDC	1651577
Pearson symbol	tP5
Space group number	99
Space group symbol	$P4mm$
AFLOW prototype command	`aflow --proto=A3BC_tP5_99_ac_b_a-002 --params=`$a, c/a, z_1, z_2, z_3, z_4$

- This is a tetragonal ferroelectric distortion of the cubic perovskite structure, $E2_1$. In $Pb(Zr_xTi_{1-x})O_3$ (aka PZT) it is found for $x \leq 0.52$. Although the first (2b) site is nearly equally occupied by zirconium and titanium atoms, the pictures use Zr atoms. Compare this to the monoclinic PZT structure.
- To recover the cubic perovskite structure, take $c = a,\ z_1 = 0,\ z_2 = 1/2,\ z_3 = 0,\ z_4 = 1/2$.

- This structure has the same space group and occupied Wyckoff positions as the tetragonal $BaTiO_3$ structure, but the displacements from the cubic perovskite structure are different, so we give this structure its own AFLOW designation.
- The ICSD lists numerous alloys in this structure, and a few ordered compounds. We have collected the ordered compounds under the room temperature $BaTiO_3$ prototype.

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)	Zr 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)	Pb 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

References

[1] B. Noheda, J. A. Gonzalo, L. E. Cross, R. Guo, S.-E. Park, D. E. Cox, and G. Shirane, *Tetragonal-to-monoclinic phase transition in a ferroelectric perovskite: The structure of* $PbZr_{0.52}Ti_{0.48}O_3$, Phys. Rev. B **61**, 8687–8695 (2000), doi:10.1103/PhysRevB.61.8687.

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