Monoclinic PZT [$Pb(Zr_xTi_{1-x})O_3$] Structure: A3BC_mC10_8_ab_a_a-001

This structure previously used the label(s) `A3BC_mC10_8_ab_a_a`. Calls to these addresses will be redirected here.

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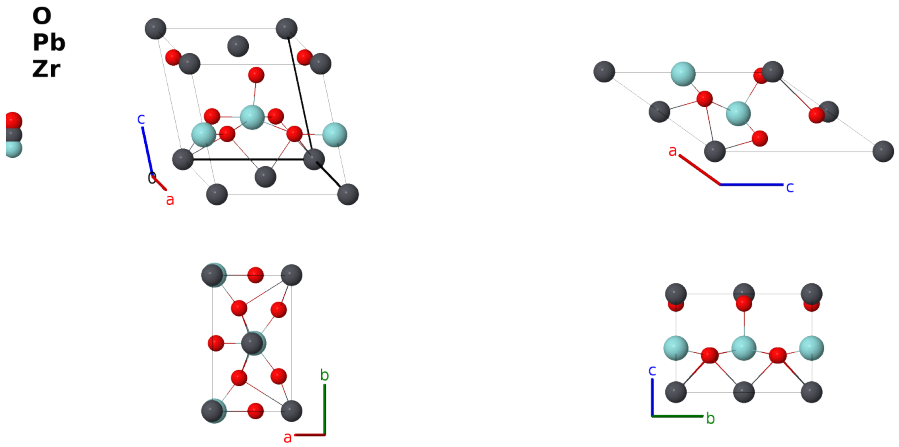
https://aflow.org/prototype-encyclopedia/XHKF

https://aflow.org/prototype-encyclopedia/A3BC_mC10_8_ab_a_a-001

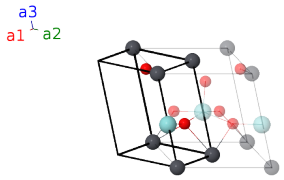


Prototype	O_3PbZr
AFLOW prototype label	A3BC_mC10_8_ab_a_a-001
Mineral name	'PZT'
ICSD	92061
CCDC	1651579
Pearson symbol	mC10
Space group number	8
Space group symbol	Cm
AFLOW prototype command	`aflow --proto=A3BC_mC10_8_ab_a_a-001 --params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, y_4, z_4$

- This is a monoclinic ferroelectric distortion of the cubic perovskite structure, $E2_1$. In $Pb(Zr_xTi_{1-x})O_3$ (aka PZT) it is found only when $x = 0.52$. Although the second (2a) site is nearly equally occupied by zirconium and titanium atoms, the pictures use Zr atoms. Compare this to the tetragonal PZT structure.

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(2a)	Pb I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(2a)	Zr I
$\mathbf{B_4}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B_5}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4b)	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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