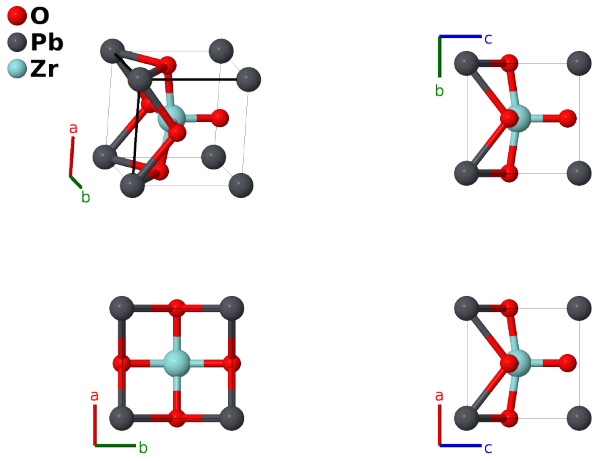
# Tetragonal PZT [$Pb(Zr_xTi_{1-x})O_3$] Structure: A3BC_tP5_99_ac_b_a-002

This structure originally had the label `A3BC_tP5_99_bc_a_b`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/Z2SB

https://aflow.org/p/A3BC_tP5_99_ac_b_a-002

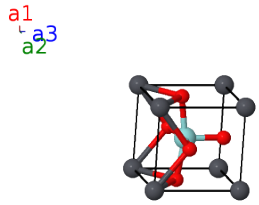



| | |
|---|---|
| **Prototype** | $O_3PbZr$ |
| **AFLOW prototype label** | A3BC_tP5_99_ac_b_a-002 |
| **Mineral name** | 'PZT' |
| **ICSD** | 92059 |
| **Pearson symbol** | tP5 |
| **Space group number** | 99 |
| **Space group symbol** | $P4mm$ |
| **AFLOW prototype command** | `aflow --proto=A3BC_tP5_99_ac_b_a-002 --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 $c = a,\ z_1 = 0,\ z_2 = 1/2,\ z_3 = 0,\ z_4 = 1/2$.

**Simple Tetragonal primitive vectors**

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$

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**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.