

ZrO₂ (High-temperature) Structure:

A2B_tP6_137_d_a-001

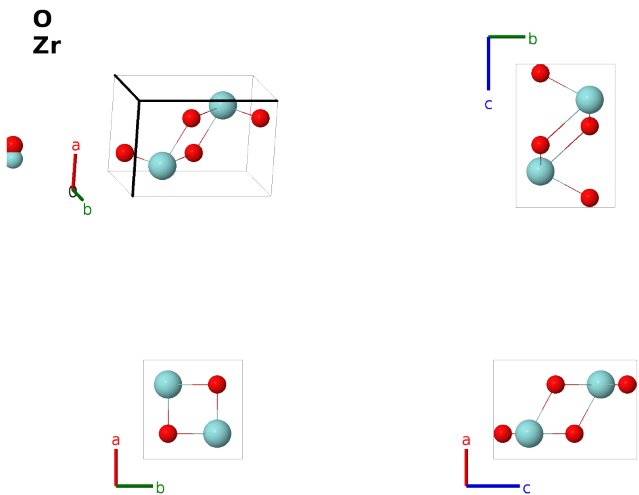
This structure previously used the label(s) **A2B_tP6_137_d_a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/T9FR>

https://aflow.org/prototype-encyclopedia/A2B_tP6_137_d_a-001



Prototype	O ₂ Zr
AFLOW prototype label	A2B_tP6_137_d_a-001
ICSD	23928
CCDC	1599988
Pearson symbol	tP6
Space group number	137
Space group symbol	$P4_2/nmc$
AFLOW prototype command	<code>aflow --proto=A2B_tP6_137_d_a-001 --params=a, c/a, z₂</code>

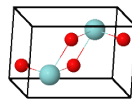
- ZrO₂ (A2B_tP6_137_d_a) and HgI₂ (AB2_tP6_137_a_d) have similar AFLOW prototype labels (i.e., same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters (**--params**) specified in their corresponding CIF files

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
$\mathbf{B}_1$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2a)	Zr I
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2a)	Zr I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4d)	O I
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	O I
$\mathbf{B}_5$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4d)	O I
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	O I

References

- [1] G. Teufer, *The crystal structure of tetragonal ZrO₂*, Acta Cryst. **15**, 1187 (1962), doi:10.1107/S0365110X62003114.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

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