ZrO_2 Structure: A2B_oP12_29_2a_a-001

This structure originally had the label `A2B_oP12_29_2a_a`. Calls to that address will be redirected here.

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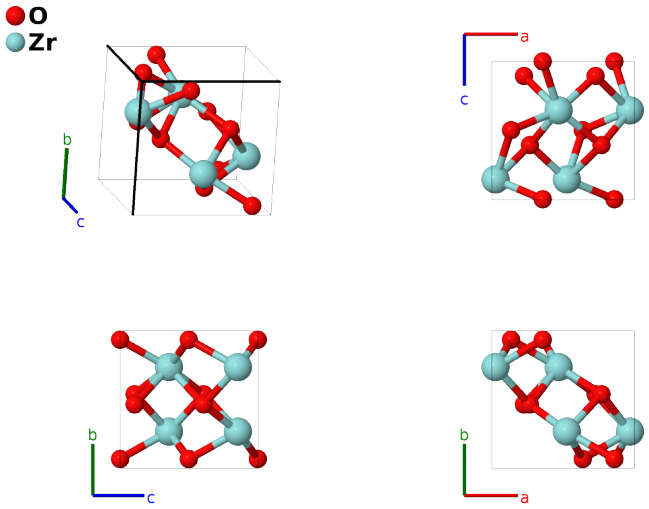
https://aflow.org/p/UZKW

https://aflow.org/p/A2B_oP12_29_2a_a-001

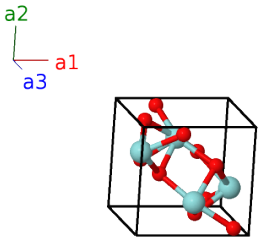


Prototype	O_2Zr
AFLOW prototype label	A2B_oP12_29_2a_a-001
ICSD	none
Pearson symbol	oP12
Space group number	29
Space group symbol	$Pca2_1$
AFLOW prototype command	`aflow --proto=A2B_oP12_29_2a_a-001 --params=`$a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3$

- The actual composition of this sample is $(Zr_{0.4}Ta_{0.6})(O_{0.7}N_{0.3})_2$.
- ZrO_2 (A2B_oP12_29_2a_a) and Pyrite (AB2_oP12_29_a_2a) 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.
- ZrO_2 is also found as baddeleyite, $C43$.

Simple Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_3}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_4}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_7}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_8}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	Zr I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Zr I
$\mathbf{B_{11}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	Zr I
$\mathbf{B_{12}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Zr I

References

[1] J. Grins, P.-O. Käll, and G. Svensson, *Phases in the $Zr_xTa_{1-x}(O,N)_y$ system, formed by ammonolysis of Zr-Ta gels: preparation of a baddeleyite-type solid solution phase $Zr_xTa_{1-x}O_{1+x}N_{1-x}$*, 0
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*le*1, J. Mater. Chem. **4**, 1293–1301 (1994), doi:10.1039/JM9940401293.

Found in

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