γ-$SrZrO_3$ Tetragonal Perovskite Structure: A3BC_tI20_140_ah_b_c-002

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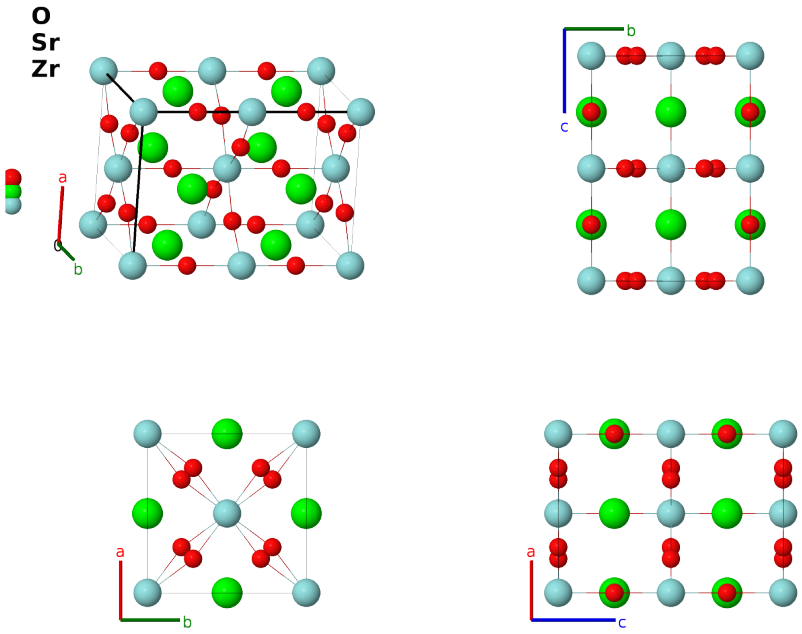
https://aflow.org/prototype-encyclopedia/AFN9

https://aflow.org/prototype-encyclopedia/A3BC_tI20_140_ah_b_c-002



Prototype	O_3SrZr
AFLOW prototype label	A3BC_tI20_140_ah_b_c-002
ICSD	89356
CCDC	1649028
Pearson symbol	tI20
Space group number	140
Space group symbol	$I4/mcm$
AFLOW prototype command	`aflow --proto=A3BC_tI20_140_ah_b_c-002 --params=`$a, c/a, x_4$

Other compounds with this structure

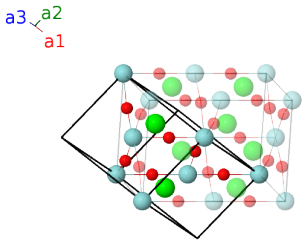
$AsNCr_3$, $BaIrO_3$, $BaPbO_3$, $BaTbO_3$, $CaTiO_3$, $CeAlO_3$, $EuNbO_3$, $EuTiO_3$, $GeCMn_3$, $KMnF_3$, $RbCaF_3$, $RuZrO_3$, $SrHfO_3$, $SrMoO_3$, $SrRuO_3$, $SrSnO_3$, $SrTcO_3$, $SrTiO_3$, $Ba(Bi, In)O_3$, $Ba(Er, Mo)O_3$, $Ba(Ho, Mn)O_3$, $Sr(Mn, Nb)O_3$, $Sr(Mn, Ru)O_3$, $Sr(Mn, Sb)O_3$, $Sr(Ru, Ti)O_3$, $Sr(Ti, Zr)O_3$, $(Ba, Ca)SrO_3$, $(Ba, Sr)HfO_3$, $(Ca, Sr)TiO_3$, $(K, Sr)BiO_3$, $(La, Sr)MnO_3$, $(Pr, Sr)MnO_3$

- As with most perovskites, $SrZrO_3$ undergoes a number of phase transitions. The temperature-driven phase transitions are summarized by (Kumar, 2017).
- We have arbitrarily labeled the phases from low- to high-temperature by Greek letters.
  - Below 970K α-$SrZrO_3$ is in the orthorhombic $CaTiO_3$ ($Pnma$) structure.
  - In the range 970-1100K, the system is in either the
    - Base-centered orthorhombic β-$SrZrO_3$ phase in the $Cmcm$ lueshite structure, or
    - The body-centered orthorhombic β'-$SrZrO_3$ phase in the orthorhombic $BaPbO_3$ structure.

    The former phase seems to be favored by experiment, but it does not share any subgroups with the $Pnma$ structure, so a direct phase transition is difficult. On the other hand the later structure does not show up in the experimental results in the ICSD, only in a theoretical calculation (ICSD 89356) by (Liu, 2012). (Kumar, 2017) mostly favor the first option, while (Fujimori, 2004) favor the second, albeit with no experimental data for the $Imma$ phase.
  - Between 1100-1440K the system is in the tetragonal γ-$SrZrO_3$ phase. (this structure)
  - Above 1440K the system is in the cubic perovskite phase ($E2_1$).
- Here we use the data taken by (Kennedy, 1999) at 1023K.
- The current structure can be a high-temperature (*e.g.* $SrZrO_3$) or high-pressure ($BaIrO_3$) phase, depending on the compound.
- We attempted to list the chemical formulas for the similar structures in the form ABC_3, where "A" is the (4b) Wyckoff position, (corresponding to the Ca site in cubic perovskite), "B" (4c) (Ti site) and "C" is (4a)&(8h) (the oxygen site).
- In addition, both the "A" (4b) and "B" (4c) sites are often alloyed, and even the (4a) and (8h) sites can be a mixture of oxygen and nitrogen.

Body-centered Tetragonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	Sr I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	Sr I
$\mathbf{B_5}$	=	0	=	0	(4c)	Zr I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	Zr I
$\mathbf{B_7}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(2x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_8}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - \left(2x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	O II

$$\mathbf{B_9} = x_4\,\mathbf{a}_1 - \left(x_4 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 = -a\left(x_4 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + a x_4\,\hat{\mathbf{y}} \quad \text{(8h)} \quad \text{O II}$$

$$\mathbf{B_{10}} = -x_4\,\mathbf{a}_1 + \left(x_4 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 = a\left(x_4 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - a x_4\,\hat{\mathbf{y}} \quad \text{(8h)} \quad \text{O II}$$

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