

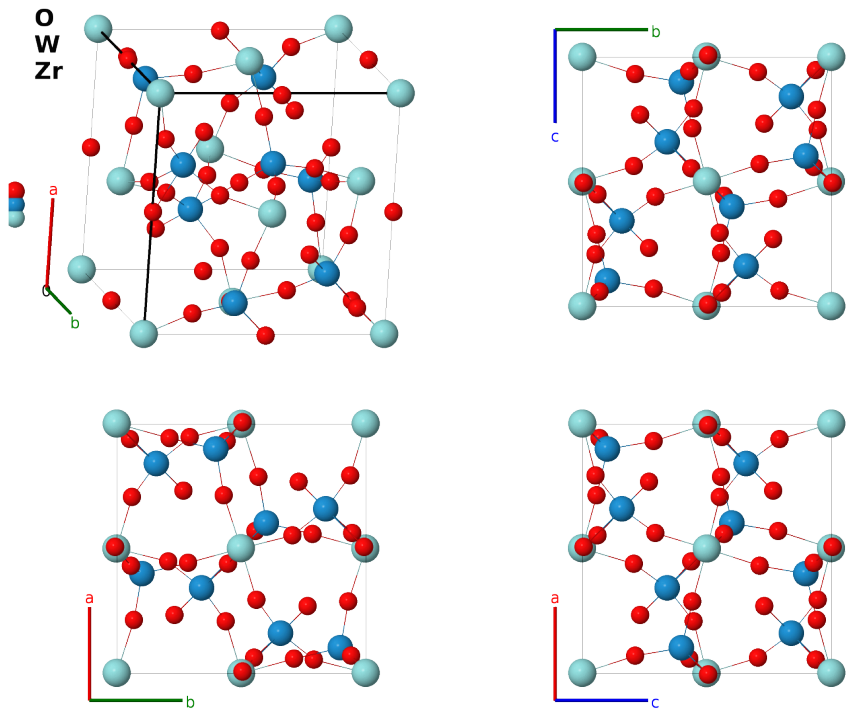
Low-Temperature ZrW_2O_8 Structure: A8B2C_cP44_198_2a2b_2a_a-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/XVW1>

https://aflow.org/prototype-encyclopedia/A8B2C_cP44_198_2a2b_2a_a-001



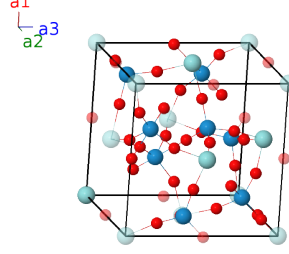
Prototype	$\text{O}_8\text{W}_2\text{Zr}$
AFLOW prototype label	A8B2C_cP44_198_2a2b_2a_a-001
ICSD	262061
CCDC	1719774
Pearson symbol	cP44
Space group number	198
Space group symbol	$P2_13$
AFLOW prototype command	<pre>aflow --proto=A8B2C_cP44_198_2a2b_2a_a-001 --params=a, x1, x2, x3, x4, x5, x6, y6, z6, x7, y7, z7</pre>

- Unusually, both ZrW_2O_8 and HfW_2O_8 have a negative thermal expansion over temperatures ranging from 0.3K to 693K. (Evans, 1996)

- Below $\approx 423\text{K}$ these compounds are in this low-temperature ZrW_2O_8 structure, sometimes referred to as $\alpha\text{-ZrW}_2\text{O}_8$.
- Above the transition the compounds are in the somewhat disordered high-temperature (β) ZrW_2O_8 structure.
- We use the data taken for LT ZrW_2O_8 at 293K .

Simple Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B}_6$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(4a)	W I
$\mathbf{B}_{10}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	W I
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	W I
$\mathbf{B}_{12}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(4a)	W I
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(4a)	W II
$\mathbf{B}_{14}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	W II
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	W II
$\mathbf{B}_{16}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(4a)	W II
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(4a)	Zr I
$\mathbf{B}_{18}$	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Zr I

$\mathbf{B}_{19} =$	$-x_5 \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_5 \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Zr I
	$(x_5 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{20} =$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(4a)	Zr I
$\mathbf{B}_{21} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{22} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 +$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + a(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O III
	$(z_6 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{23} =$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_6 \hat{\mathbf{x}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O III
	$(z_6 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{24} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{25} =$	$z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$az_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{26} =$	$(z_6 + \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$a(z_6 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{27} =$	$-(z_6 - \frac{1}{2}) \mathbf{a}_1 - x_6 \mathbf{a}_2 +$	$=$	$-a(z_6 - \frac{1}{2}) \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O III
	$(y_6 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{28} =$	$-z_6 \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-az_6 \hat{\mathbf{x}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O III
	$(y_6 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{29} =$	$y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}} + ax_6 \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{30} =$	$-y_6 \mathbf{a}_1 + (z_6 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ay_6 \hat{\mathbf{x}} + a(z_6 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O III
	$(x_6 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{31} =$	$(y_6 + \frac{1}{2}) \mathbf{a}_1 - (z_6 - \frac{1}{2}) \mathbf{a}_2 - x_6 \mathbf{a}_3$	$=$	$a(y_6 + \frac{1}{2}) \hat{\mathbf{x}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{32} =$	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 - z_6 \mathbf{a}_2 +$	$=$	$-a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O III
	$(x_6 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{33} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + az_7 \hat{\mathbf{z}}$	(12b)	O IV
$\mathbf{B}_{34} =$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 - y_7 \mathbf{a}_2 +$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + a(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O IV
	$(z_7 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{35} =$	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_7 \hat{\mathbf{x}} + a(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O IV
	$(z_7 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{36} =$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - az_7 \hat{\mathbf{z}}$	(12b)	O IV
$\mathbf{B}_{37} =$	$z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + y_7 \mathbf{a}_3$	$=$	$az_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + ay_7 \hat{\mathbf{z}}$	(12b)	O IV
$\mathbf{B}_{38} =$	$(z_7 + \frac{1}{2}) \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 - y_7 \mathbf{a}_3$	$=$	$a(z_7 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{y}} - ay_7 \hat{\mathbf{z}}$	(12b)	O IV
$\mathbf{B}_{39} =$	$-(z_7 - \frac{1}{2}) \mathbf{a}_1 - x_7 \mathbf{a}_2 +$	$=$	$-a(z_7 - \frac{1}{2}) \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + a(y_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O IV
	$(y_7 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{40} =$	$-z_7 \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-az_7 \hat{\mathbf{x}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O IV
	$(y_7 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{41} =$	$y_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} + az_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(12b)	O IV
$\mathbf{B}_{42} =$	$-y_7 \mathbf{a}_1 + (z_7 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ay_7 \hat{\mathbf{x}} + a(z_7 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O IV
	$(x_7 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{43} =$	$(y_7 + \frac{1}{2}) \mathbf{a}_1 - (z_7 - \frac{1}{2}) \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$a(y_7 + \frac{1}{2}) \hat{\mathbf{x}} - a(z_7 - \frac{1}{2}) \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(12b)	O IV
$\mathbf{B}_{44} =$	$-(y_7 - \frac{1}{2}) \mathbf{a}_1 - z_7 \mathbf{a}_2 +$	$=$	$-a(y_7 - \frac{1}{2}) \hat{\mathbf{x}} - az_7 \hat{\mathbf{y}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O IV
	$(x_7 + \frac{1}{2}) \mathbf{a}_3$				

References

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