

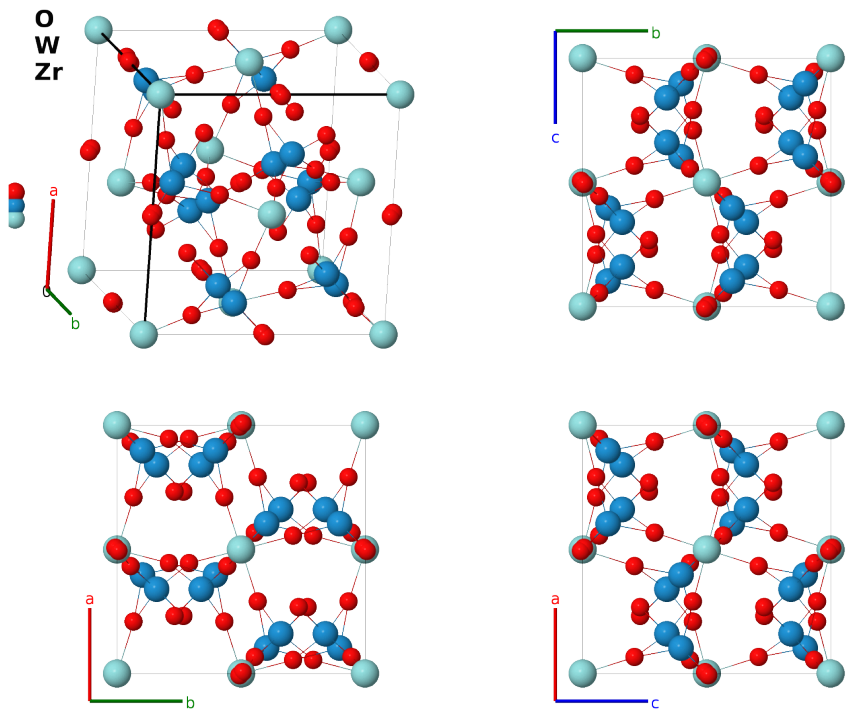
High-Temperature ZrW_2O_8 Structure: A10B4C_cP60_205_2cd_2c_a-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/SZRA>

https://aflow.org/prototype-encyclopedia/A10B4C_cP60_205_2cd_2c_a-001



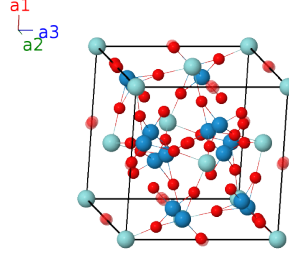
Prototype	$\text{O}_8\text{W}_2\text{Zr}$
AFLOW prototype label	A10B4C_cP60_205_2cd_2c_a-001
ICSD	262062
CCDC	1719774
Pearson symbol	cP60
Space group number	205
Space group symbol	$P\bar{a}3$
AFLOW prototype command	<code>aflow --proto=A10B4C_cP60_205_2cd_2c_a-001</code> <code>--params=a, x2, x3, x4, x5, x6, y6, z6</code>

Other compounds with this structure
 HfW_2O_8

- 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 the low-temperature ZrW_2O_8 structure, sometimes referred to as $\alpha\text{-ZrW}_2\text{O}_8$.
- Above the transition the compounds are in this somewhat disordered high-temperature (β) ZrW_2O_8 structure.
- In this high-temperature phase all of the (8c) sites are only 50% occupied. Only one of each conjoined pair of atoms in the diagram will be present in a real sample.

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
$\mathbf{B}_1$	$= 0$	$=$	0	(4a)	Zr I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4a)	Zr I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(4a)	Zr I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(4a)	Zr I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_6$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_9$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_{10}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + x_2 \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_{11}$	$= x_2 \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_{12}$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_{13}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{14}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{15}$	$= -x_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{16}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{17}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{18}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O II

$\mathbf{B}_{19} =$	$x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{20} =$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 +$ $x_3 \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{21} =$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(8c)	W I
$\mathbf{B}_{22} =$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 - x_4 \mathbf{a}_2 +$ $(x_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	W I
$\mathbf{B}_{23} =$	$-x_4 \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 -$ $(x_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	W I
$\mathbf{B}_{24} =$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(8c)	W I
$\mathbf{B}_{25} =$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(8c)	W I
$\mathbf{B}_{26} =$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 + x_4 \mathbf{a}_2 - (x_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	W I
$\mathbf{B}_{27} =$	$x_4 \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + (x_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	W I
$\mathbf{B}_{28} =$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 +$ $x_4 \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(8c)	W I
$\mathbf{B}_{29} =$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(8c)	W II
$\mathbf{B}_{30} =$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 - x_5 \mathbf{a}_2 +$ $(x_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	W II
$\mathbf{B}_{31} =$	$-x_5 \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 -$ $(x_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	W II
$\mathbf{B}_{32} =$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(8c)	W II
$\mathbf{B}_{33} =$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(8c)	W II
$\mathbf{B}_{34} =$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 + x_5 \mathbf{a}_2 - (x_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	W II
$\mathbf{B}_{35} =$	$x_5 \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + (x_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	W II
$\mathbf{B}_{36} =$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 +$ $x_5 \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(8c)	W II
$\mathbf{B}_{37} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}}$	(24d)	O III
$\mathbf{B}_{38} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 +$ $(z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + a(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(24d)	O III
$\mathbf{B}_{39} =$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 -$ $(z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(24d)	O III
$\mathbf{B}_{40} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}}$	(24d)	O III
$\mathbf{B}_{41} =$	$z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$az_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}}$	(24d)	O III
$\mathbf{B}_{42} =$	$(z_6 + \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$a(z_6 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}}$	(24d)	O III
$\mathbf{B}_{43} =$	$-(z_6 - \frac{1}{2}) \mathbf{a}_1 - x_6 \mathbf{a}_2 +$ $(y_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(z_6 - \frac{1}{2}) \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(24d)	O III
$\mathbf{B}_{44} =$	$-z_6 \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 -$ $(y_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-az_6 \hat{\mathbf{x}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(24d)	O III
$\mathbf{B}_{45} =$	$y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}} + ax_6 \hat{\mathbf{z}}$	(24d)	O III
$\mathbf{B}_{46} =$	$-y_6 \mathbf{a}_1 + (z_6 + \frac{1}{2}) \mathbf{a}_2 -$ $(x_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + a(z_6 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(24d)	O III
$\mathbf{B}_{47} =$	$(y_6 + \frac{1}{2}) \mathbf{a}_1 - (z_6 - \frac{1}{2}) \mathbf{a}_2 - x_6 \mathbf{a}_3$	$=$	$a(y_6 + \frac{1}{2}) \hat{\mathbf{x}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}}$	(24d)	O III
$\mathbf{B}_{48} =$	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 - z_6 \mathbf{a}_2 +$ $(x_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(24d)	O III
$\mathbf{B}_{49} =$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}}$	(24d)	O III

$$\begin{aligned}
\mathbf{B}_{50} &= (x_6 + \tfrac{1}{2}) \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \tfrac{1}{2}) \mathbf{a}_3 = a(x_6 + \tfrac{1}{2}) \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} - a(z_6 - \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O III} \\
\mathbf{B}_{51} &= x_6 \mathbf{a}_1 - (y_6 - \tfrac{1}{2}) \mathbf{a}_2 + (z_6 + \tfrac{1}{2}) \mathbf{a}_3 = ax_6 \hat{\mathbf{x}} - a(y_6 - \tfrac{1}{2}) \hat{\mathbf{y}} + a(z_6 + \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O III} \\
\mathbf{B}_{52} &= -(x_6 - \tfrac{1}{2}) \mathbf{a}_1 + (y_6 + \tfrac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3 = -a(x_6 - \tfrac{1}{2}) \hat{\mathbf{x}} + a(y_6 + \tfrac{1}{2}) \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}} & (24d) & \text{O III} \\
\mathbf{B}_{53} &= -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}} & (24d) & \text{O III} \\
\mathbf{B}_{54} &= -(z_6 - \tfrac{1}{2}) \mathbf{a}_1 + (x_6 + \tfrac{1}{2}) \mathbf{a}_2 + y_6 \mathbf{a}_3 = -a(z_6 - \tfrac{1}{2}) \hat{\mathbf{x}} + a(x_6 + \tfrac{1}{2}) \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}} & (24d) & \text{O III} \\
\mathbf{B}_{55} &= (z_6 + \tfrac{1}{2}) \mathbf{a}_1 + x_6 \mathbf{a}_2 - (y_6 - \tfrac{1}{2}) \mathbf{a}_3 = a(z_6 + \tfrac{1}{2}) \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - a(y_6 - \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O III} \\
\mathbf{B}_{56} &= z_6 \mathbf{a}_1 - (x_6 - \tfrac{1}{2}) \mathbf{a}_2 + (y_6 + \tfrac{1}{2}) \mathbf{a}_3 = az_6 \hat{\mathbf{x}} - a(x_6 - \tfrac{1}{2}) \hat{\mathbf{y}} + a(y_6 + \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O III} \\
\mathbf{B}_{57} &= -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}} & (24d) & \text{O III} \\
\mathbf{B}_{58} &= y_6 \mathbf{a}_1 - (z_6 - \tfrac{1}{2}) \mathbf{a}_2 + (x_6 + \tfrac{1}{2}) \mathbf{a}_3 = ay_6 \hat{\mathbf{x}} - a(z_6 - \tfrac{1}{2}) \hat{\mathbf{y}} + a(x_6 + \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O III} \\
\mathbf{B}_{59} &= -(y_6 - \tfrac{1}{2}) \mathbf{a}_1 + (z_6 + \tfrac{1}{2}) \mathbf{a}_2 + x_6 \mathbf{a}_3 = -a(y_6 - \tfrac{1}{2}) \hat{\mathbf{x}} + a(z_6 + \tfrac{1}{2}) \hat{\mathbf{y}} + ax_6 \hat{\mathbf{z}} & (24d) & \text{O III} \\
\mathbf{B}_{60} &= (y_6 + \tfrac{1}{2}) \mathbf{a}_1 + z_6 \mathbf{a}_2 - (x_6 - \tfrac{1}{2}) \mathbf{a}_3 = a(y_6 + \tfrac{1}{2}) \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}} - a(x_6 - \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O III}
\end{aligned}$$

References

- [1] J. S. O. Evans, T. A. Mary, T. Vogt, M. A. Subramanian, and A. W. Sleight, *Negative Thermal Expansion in ZrW_2O_8 and HfW_2O_8* , Chem. Mater. **8**, 2809–2823 (1996), doi:10.1021/cm9602959.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).