Low Temperature CsW_2O_6 Structure: AB6C2_cP72_198_2a_4b_ab-001

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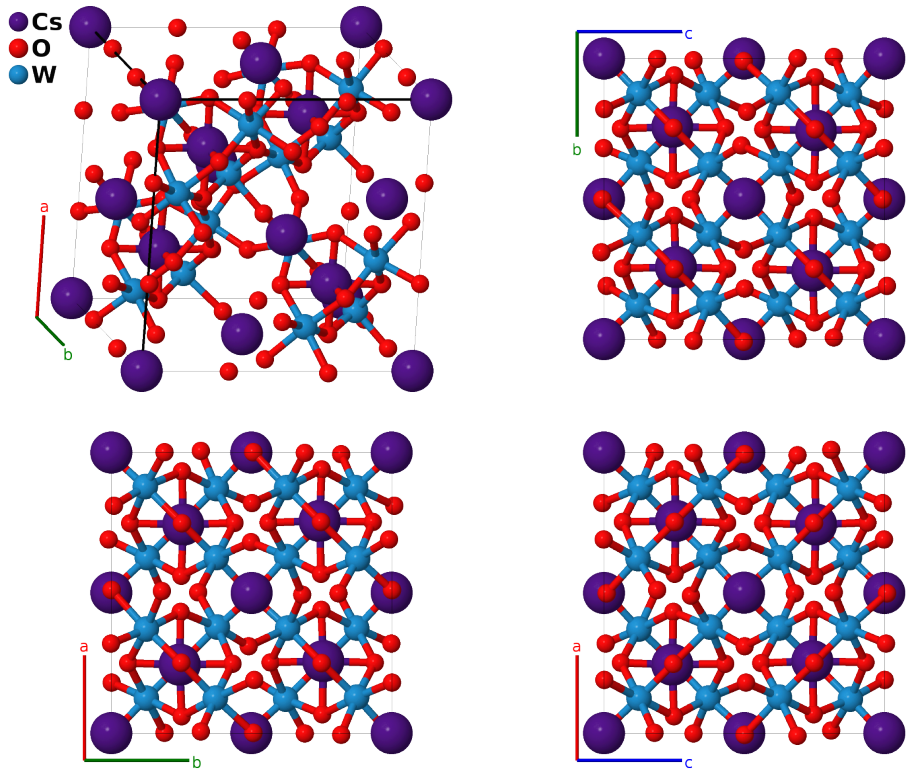
https://aflow.org/p/WBDQ

https://aflow.org/p/AB6C2_cP72_198_2a_4b_ab-001

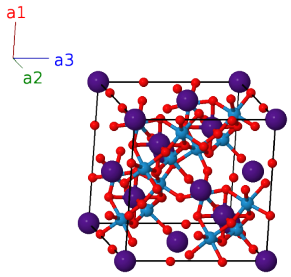


Prototype	CsO_6W_2
AFLOW prototype label	AB6C2_cP72_198_2a_4b_ab-001
ICSD	none
Pearson symbol	cP72
Space group number	198
Space group symbol	$P2_13$
AFLOW prototype command	`aflow --proto=AB6C2_cP72_198_2a_4b_ab-001 --params=`$a, x_1, x_2, x_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

- This is the ground state structure of CsW_2O_6, with data taken at 100K. Above 215K this transforms into the cubic (or β-) pyrochlore structure, $E8_1$.

Simple Cubic primitive vectors

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



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)	Cs 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)	Cs 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)	Cs 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)	Cs 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)	Cs 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)	Cs 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)	Cs 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)	Cs 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
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} + a\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{16}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{17}}$	=	$z_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$az_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ay_4\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{18}}$	=	$\left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$a\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - ay_4\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{19}}$	=	$-\left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + a\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{20}}$	=	$-z_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-az_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O I
$\mathbf{B_{21}}$	=	$y_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(12b)	O I

$$
\begin{array}{lcccccc}
\mathbf{B_{22}} & = & -y_4\,\mathbf{a}_1+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ay_4\,\hat{\mathbf{x}}+a\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12b)} & \text{O I}\\
\mathbf{B_{23}} & = & \left(y_4+\frac{1}{2}\right)\,\mathbf{a}_1-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_2-x_4\,\mathbf{a}_3 & = & a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}-ax_4\,\hat{\mathbf{z}} & \text{(12b)} & \text{O I}\\
\mathbf{B_{24}} & = & -\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_1-z_4\,\mathbf{a}_2+\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}-az_4\,\hat{\mathbf{y}}+a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12b)} & \text{O I}\\
\mathbf{B_{25}} & = & x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3 & = & ax_5\,\hat{\mathbf{x}}+ay_5\,\hat{\mathbf{y}}+az_5\,\hat{\mathbf{z}} & \text{(12b)} & \text{O II}\\
\mathbf{B_{26}} & = & -\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1-y_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}+a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12b)} & \text{O II}\\
\mathbf{B_{27}} & = & -x_5\,\mathbf{a}_1+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_5\,\hat{\mathbf{x}}+a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12b)} & \text{O II}\\
\mathbf{B_{28}} & = & \left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2-z_5\,\mathbf{a}_3 & = & a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}-az_5\,\hat{\mathbf{z}} & \text{(12b)} & \text{O II}\\
\mathbf{B_{29}} & = & z_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+y_5\,\mathbf{a}_3 & = & az_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}+ay_5\,\hat{\mathbf{z}} & \text{(12b)} & \text{O II}\\
\mathbf{B_{30}} & = & \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2-y_5\,\mathbf{a}_3 & = & a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}-ay_5\,\hat{\mathbf{z}} & \text{(12b)} & \text{O II}\\
\mathbf{B_{31}} & = & -\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_1-x_5\,\mathbf{a}_2+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12b)} & \text{O II}\\
\mathbf{B_{32}} & = & -z_5\,\mathbf{a}_1+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_2-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_3 & = & -az_5\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12b)} & \text{O II}\\
\mathbf{B_{33}} & = & y_5\,\mathbf{a}_1+z_5\,\mathbf{a}_2+x_5\,\mathbf{a}_3 & = & ay_5\,\hat{\mathbf{x}}+az_5\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}} & \text{(12b)} & \text{O II}\\
\mathbf{B_{34}} & = & -y_5\,\mathbf{a}_1+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ay_5\,\hat{\mathbf{x}}+a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12b)} & \text{O II}\\
\mathbf{B_{35}} & = & \left(y_5+\frac{1}{2}\right)\,\mathbf{a}_1-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_2-x_5\,\mathbf{a}_3 & = & a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}} & \text{(12b)} & \text{O II}\\
\mathbf{B_{36}} & = & -\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_1-z_5\,\mathbf{a}_2+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}-az_5\,\hat{\mathbf{y}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12b)} & \text{O 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}} & \text{(12b)} & \text{O III}\\
\mathbf{B_{38}} & = & -\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_1-y_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{x}}-ay_6\,\hat{\mathbf{y}}+a\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12b)} & \text{O III}\\
\mathbf{B_{39}} & = & -x_6\,\mathbf{a}_1+\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_6-\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_6\,\hat{\mathbf{x}}+a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(z_6-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12b)} & \text{O III}\\
\mathbf{B_{40}} & = & \left(x_6+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_2-z_6\,\mathbf{a}_3 & = & a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}-az_6\,\hat{\mathbf{z}} & \text{(12b)} & \text{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}} & \text{(12b)} & \text{O III}\\
\mathbf{B_{42}} & = & \left(z_6+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_2-y_6\,\mathbf{a}_3 & = & a\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}-ay_6\,\hat{\mathbf{z}} & \text{(12b)} & \text{O III}\\
\mathbf{B_{43}} & = & -\left(z_6-\frac{1}{2}\right)\,\mathbf{a}_1-x_6\,\mathbf{a}_2+\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(z_6-\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_6\,\hat{\mathbf{y}}+a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12b)} & \text{O III}\\
\mathbf{B_{44}} & = & -z_6\,\mathbf{a}_1+\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_2-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_3 & = & -az_6\,\hat{\mathbf{x}}+a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12b)} & \text{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}} & \text{(12b)} & \text{O III}\\
\mathbf{B_{46}} & = & -y_6\,\mathbf{a}_1+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ay_6\,\hat{\mathbf{x}}+a\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12b)} & \text{O III}\\
\mathbf{B_{47}} & = & \left(y_6+\frac{1}{2}\right)\,\mathbf{a}_1-\left(z_6-\frac{1}{2}\right)\,\mathbf{a}_2-x_6\,\mathbf{a}_3 & = & a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(z_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}-ax_6\,\hat{\mathbf{z}} & \text{(12b)} & \text{O III}\\
\mathbf{B_{48}} & = & -\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_1-z_6\,\mathbf{a}_2+\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{x}}-az_6\,\hat{\mathbf{y}}+a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12b)} & \text{O III}\\
\mathbf{B_{49}} & = & 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}} & \text{(12b)} & \text{O IV}\\
\mathbf{B_{50}} & = & -\left(x_7-\frac{1}{2}\right)\,\mathbf{a}_1-y_7\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{x}}-ay_7\,\hat{\mathbf{y}}+a\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(12b)} & \text{O IV}
\end{array}
$$

$$\mathbf{B_{51}} = -x_7\,\mathbf{a}_1 + \left(y_7+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_7-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} + a\left(y_7+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(z_7-\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (12b) \quad \text{O IV}$$

$$\mathbf{B_{52}} = \left(x_7+\tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(y_7-\tfrac{1}{2}\right)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = a\left(x_7+\tfrac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_7-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - az_7\,\hat{\mathbf{z}} \quad (12b) \quad \text{O IV}$$

$$\mathbf{B_{53}} = z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + y_7\,\mathbf{a}_3 = az_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + ay_7\,\hat{\mathbf{z}} \quad (12b) \quad \text{O IV}$$

$$\mathbf{B_{54}} = \left(z_7+\tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(x_7-\tfrac{1}{2}\right)\,\mathbf{a}_2 - y_7\,\mathbf{a}_3 = a\left(z_7+\tfrac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_7-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - ay_7\,\hat{\mathbf{z}} \quad (12b) \quad \text{O IV}$$

$$\mathbf{B_{55}} = -\left(z_7-\tfrac{1}{2}\right)\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + \left(y_7+\tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(z_7-\tfrac{1}{2}\right)\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + a\left(y_7+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (12b) \quad \text{O IV}$$

$$\mathbf{B_{56}} = -z_7\,\mathbf{a}_1 + \left(x_7+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(y_7-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -az_7\,\hat{\mathbf{x}} + a\left(x_7+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_7-\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (12b) \quad \text{O IV}$$

$$\mathbf{B_{57}} = y_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3 = ay_7\,\hat{\mathbf{x}} + az_7\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}} \quad (12b) \quad \text{O IV}$$

$$\mathbf{B_{58}} = -y_7\,\mathbf{a}_1 + \left(z_7+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(x_7-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -ay_7\,\hat{\mathbf{x}} + a\left(z_7+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_7-\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (12b) \quad \text{O IV}$$

$$\mathbf{B_{59}} = \left(y_7+\tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(z_7-\tfrac{1}{2}\right)\,\mathbf{a}_2 - x_7\,\mathbf{a}_3 = a\left(y_7+\tfrac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(z_7-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - ax_7\,\hat{\mathbf{z}} \quad (12b) \quad \text{O IV}$$

$$\mathbf{B_{60}} = -\left(y_7-\tfrac{1}{2}\right)\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 + \left(x_7+\tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(y_7-\tfrac{1}{2}\right)\,\hat{\mathbf{x}} - az_7\,\hat{\mathbf{y}} + a\left(x_7+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (12b) \quad \text{O IV}$$

$$\mathbf{B_{61}} = x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = ax_8\,\hat{\mathbf{x}} + ay_8\,\hat{\mathbf{y}} + az_8\,\hat{\mathbf{z}} \quad (12b) \quad \text{W II}$$

$$\mathbf{B_{62}} = -\left(x_8-\tfrac{1}{2}\right)\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8+\tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(x_8-\tfrac{1}{2}\right)\,\hat{\mathbf{x}} - ay_8\,\hat{\mathbf{y}} + a\left(z_8+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (12b) \quad \text{W II}$$

$$\mathbf{B_{63}} = -x_8\,\mathbf{a}_1 + \left(y_8+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_8-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -ax_8\,\hat{\mathbf{x}} + a\left(y_8+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(z_8-\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (12b) \quad \text{W II}$$

$$\mathbf{B_{64}} = \left(x_8+\tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(y_8-\tfrac{1}{2}\right)\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = a\left(x_8+\tfrac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_8-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - az_8\,\hat{\mathbf{z}} \quad (12b) \quad \text{W II}$$

$$\mathbf{B_{65}} = z_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + y_8\,\mathbf{a}_3 = az_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + ay_8\,\hat{\mathbf{z}} \quad (12b) \quad \text{W II}$$

$$\mathbf{B_{66}} = \left(z_8+\tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(x_8-\tfrac{1}{2}\right)\,\mathbf{a}_2 - y_8\,\mathbf{a}_3 = a\left(z_8+\tfrac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_8-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - ay_8\,\hat{\mathbf{z}} \quad (12b) \quad \text{W II}$$

$$\mathbf{B_{67}} = -\left(z_8-\tfrac{1}{2}\right)\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + \left(y_8+\tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(z_8-\tfrac{1}{2}\right)\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} + a\left(y_8+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (12b) \quad \text{W II}$$

$$\mathbf{B_{68}} = -z_8\,\mathbf{a}_1 + \left(x_8+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(y_8-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -az_8\,\hat{\mathbf{x}} + a\left(x_8+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_8-\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (12b) \quad \text{W II}$$

$$\mathbf{B_{69}} = y_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3 = ay_8\,\hat{\mathbf{x}} + az_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}} \quad (12b) \quad \text{W II}$$

$$\mathbf{B_{70}} = -y_8\,\mathbf{a}_1 + \left(z_8+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(x_8-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -ay_8\,\hat{\mathbf{x}} + a\left(z_8+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_8-\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (12b) \quad \text{W II}$$

$$\mathbf{B_{71}} = \left(y_8+\tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(z_8-\tfrac{1}{2}\right)\,\mathbf{a}_2 - x_8\,\mathbf{a}_3 = a\left(y_8+\tfrac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(z_8-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}} \quad (12b) \quad \text{W II}$$

$$\mathbf{B_{72}} = -\left(y_8-\tfrac{1}{2}\right)\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 + \left(x_8+\tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(y_8-\tfrac{1}{2}\right)\,\hat{\mathbf{x}} - az_8\,\hat{\mathbf{y}} + a\left(x_8+\tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (12b) \quad \text{W II}$$

References

[1] Y. Okamoto, H. Amano, N. Katayama, H. Sawa, K. Niki, R. Mitoka, H. Harima, T. Hasegawa, N. Ogita, Y. Tanaka, M. Takigawa, Y. Yokoyama, K. Takehana, Y. Imanaka, Y. Nakamura, H. Kishida, and K. Takenaka, *Regular-triangle trimer and charge order preserving the Anderson condition in the pyrochlore structure of* CsW_2O_6, Nature Comm. **11**, 3144 (2020), doi:10.1038/s41467-020-16873-7.

Found in

[1] Y. Okamoto, *Unusual electron sharing found in cool crystal* (2020). Phys.Org.