Tetragonal Potassium Bronze ($K_3W_5O_{15}$) Structure: A3B15C5_tP46_127_bh_cg2ij_di-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

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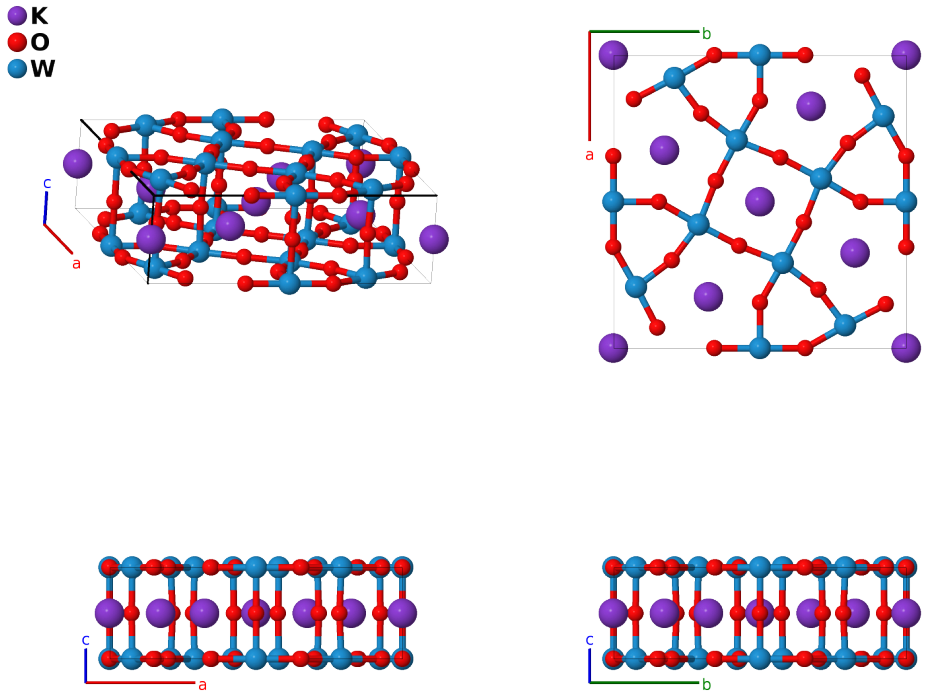


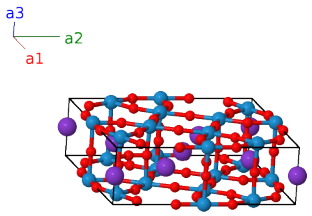
Prototype	$K_3O_{15}W_3$
AFLOW prototype label	A3B15C5_tP46_127_bh_cg2ij_di-001
Mineral name	bronze
ICSD	24730
Pearson symbol	tP46
Space group number	127
Space group symbol	$P4/mbm$
AFLOW prototype command	`aflow --proto=A3B15C5_tP46_127_bh_cg2ij_di-001 --params=`$a, c/a, x_4, x_5, x_6, y_6, x_7, y_7, x_8, y_8, x_9, y_9$

- (Hyde, 1973) notes that this is a derivative of the α-ReO_3 ($D0_9$) structure.
- The measured structure is actually deficient in potassium. We use the lattice constants from (Magnéli, 1949) for $K_{0.57}WO_3$.

- Magnéli's X-ray data could not determine the oxygen positions. The coordinates for the oxygen atoms were determined by the requirement that the space group be $P4/mbm$ #127. as determined by the positions of the potassium and tungsten atoms, and by "considerations of space."

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	K I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	K I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(2d)	W I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2d)	W I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B_9}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B_{10}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B_{11}}$	=	$x_5\,\mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	K II
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	K II
$\mathbf{B_{13}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	K II
$\mathbf{B_{14}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	K II
$\mathbf{B_{15}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2$	=	$ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}}$	(8i)	O III
$\mathbf{B_{16}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2$	=	$-ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}}$	(8i)	O III
$\mathbf{B_{17}}$	=	$-y_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2$	=	$-ay_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}}$	(8i)	O III
$\mathbf{B_{18}}$	=	$y_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2$	=	$ay_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}}$	(8i)	O III
$\mathbf{B_{19}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8i)	O III
$\mathbf{B_{20}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8i)	O III
$\mathbf{B_{21}}$	=	$\left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$a\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8i)	O III
$\mathbf{B_{22}}$	=	$-\left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-a\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8i)	O III
$\mathbf{B_{23}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2$	=	$ax_7\,\hat{\mathbf{x}} + ay_7\,\hat{\mathbf{y}}$	(8i)	O IV
$\mathbf{B_{24}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2$	=	$-ax_7\,\hat{\mathbf{x}} - ay_7\,\hat{\mathbf{y}}$	(8i)	O IV
$\mathbf{B_{25}}$	=	$-y_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2$	=	$-ay_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}}$	(8i)	O IV
$\mathbf{B_{26}}$	=	$y_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2$	=	$ay_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}}$	(8i)	O IV

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\begin{array}{rcccccc}
\mathbf{B_{27}} & = & -\left(x_7-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_7+\frac{1}{2}\right)\,\mathbf{a}_2 & = & -a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_7+\frac{1}{2}\right)\,\hat{\mathbf{y}} & \text{(8i)} & \text{O IV}\\
\mathbf{B_{28}} & = & \left(x_7+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_7-\frac{1}{2}\right)\,\mathbf{a}_2 & = & a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{y}} & \text{(8i)} & \text{O IV}\\
\mathbf{B_{29}} & = & \left(y_7+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_7+\frac{1}{2}\right)\,\mathbf{a}_2 & = & a\left(y_7+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{y}} & \text{(8i)} & \text{O IV}\\
\mathbf{B_{30}} & = & -\left(y_7-\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_7-\frac{1}{2}\right)\,\mathbf{a}_2 & = & -a\left(y_7-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{y}} & \text{(8i)} & \text{O IV}\\
\mathbf{B_{31}} & = & x_8\,\mathbf{a}_1+y_8\,\mathbf{a}_2 & = & ax_8\,\hat{\mathbf{x}}+ay_8\,\hat{\mathbf{y}} & \text{(8i)} & \text{W II}\\
\mathbf{B_{32}} & = & -x_8\,\mathbf{a}_1-y_8\,\mathbf{a}_2 & = & -ax_8\,\hat{\mathbf{x}}-ay_8\,\hat{\mathbf{y}} & \text{(8i)} & \text{W II}\\
\mathbf{B_{33}} & = & -y_8\,\mathbf{a}_1+x_8\,\mathbf{a}_2 & = & -ay_8\,\hat{\mathbf{x}}+ax_8\,\hat{\mathbf{y}} & \text{(8i)} & \text{W II}\\
\mathbf{B_{34}} & = & y_8\,\mathbf{a}_1-x_8\,\mathbf{a}_2 & = & ay_8\,\hat{\mathbf{x}}-ax_8\,\hat{\mathbf{y}} & \text{(8i)} & \text{W II}\\
\mathbf{B_{35}} & = & -\left(x_8-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_8+\frac{1}{2}\right)\,\mathbf{a}_2 & = & -a\left(x_8-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_8+\frac{1}{2}\right)\,\hat{\mathbf{y}} & \text{(8i)} & \text{W II}\\
\mathbf{B_{36}} & = & \left(x_8+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_8-\frac{1}{2}\right)\,\mathbf{a}_2 & = & a\left(x_8+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_8-\frac{1}{2}\right)\,\hat{\mathbf{y}} & \text{(8i)} & \text{W II}\\
\mathbf{B_{37}} & = & \left(y_8+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_8+\frac{1}{2}\right)\,\mathbf{a}_2 & = & a\left(y_8+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_8+\frac{1}{2}\right)\,\hat{\mathbf{y}} & \text{(8i)} & \text{W II}\\
\mathbf{B_{38}} & = & -\left(y_8-\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_8-\frac{1}{2}\right)\,\mathbf{a}_2 & = & -a\left(y_8-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_8-\frac{1}{2}\right)\,\hat{\mathbf{y}} & \text{(8i)} & \text{W II}\\
\mathbf{B_{39}} & = & x_9\,\mathbf{a}_1+y_9\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3 & = & ax_9\,\hat{\mathbf{x}}+ay_9\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}} & \text{(8j)} & \text{O V}\\
\mathbf{B_{40}} & = & -x_9\,\mathbf{a}_1-y_9\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3 & = & -ax_9\,\hat{\mathbf{x}}-ay_9\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}} & \text{(8j)} & \text{O V}\\
\mathbf{B_{41}} & = & -y_9\,\mathbf{a}_1+x_9\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3 & = & -ay_9\,\hat{\mathbf{x}}+ax_9\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}} & \text{(8j)} & \text{O V}\\
\mathbf{B_{42}} & = & y_9\,\mathbf{a}_1-x_9\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3 & = & ay_9\,\hat{\mathbf{x}}-ax_9\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}} & \text{(8j)} & \text{O V}\\
\mathbf{B_{43}} & = & -\left(x_9-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_9+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3 & = & -a\left(x_9-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_9+\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}} & \text{(8j)} & \text{O V}\\
\mathbf{B_{44}} & = & \left(x_9+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_9-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3 & = & a\left(x_9+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_9-\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}} & \text{(8j)} & \text{O V}\\
\mathbf{B_{45}} & = & \left(y_9+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_9+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3 & = & a\left(y_9+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_9+\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}} & \text{(8j)} & \text{O V}\\
\mathbf{B_{46}} & = & -\left(y_9-\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_9-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3 & = & -a\left(y_9-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_9-\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}} & \text{(8j)} & \text{O V}
\end{array}
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References

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[2] B. G. Hyde and M. O'Keefe, *Relations between the $DO_9(ReO_3)$ structure type and some "bronze" and "tunnel" structures*, Acta Crystallogr. Sect. A **29**, 243–248 (1973), doi:10.1107/S056773947300063X.

Found in

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