

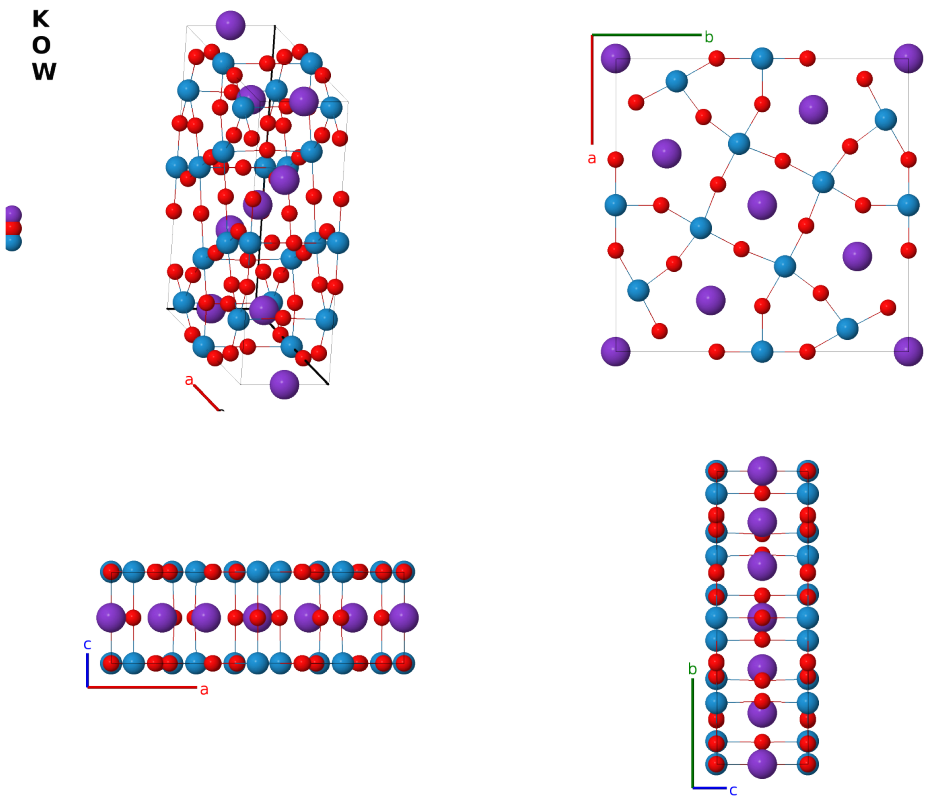
Tetragonal Potassium Bronze ($K_3W_5O_{15}$) Structure: A3B15C5_tP46_127_bh_cg2ij_di-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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. Oses, 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/LCR4>

https://aflow.org/prototype-encyclopedia/A3B15C5_tP46_127_bh_cg2ij_di-001

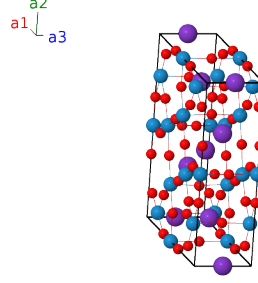


Prototype	$K_3O_{15}W_3$
AFLOW prototype label	A3B15C5_tP46_127_bh_cg2ij_di-001
Mineral name	bronze
ICSD	24730
CCDC	1600742
Pearson symbol	tP46
Space group number	127
Space group symbol	$P4/mbm$
AFLOW prototype command	<code>aflow --proto=A3B15C5_tP46_127_bh_cg2ij_di-001</code> <code>--params=a, c/a, x_4, x_5, x_6, y_6, x_7, y_7, x_8, y_8, x_9, y_9</code>

- (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 $\text{K}_{0.57}\text{WO}_3$.
- 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

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



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
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B}_9$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + x_4 \mathbf{a}_2$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B}_{10}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B}_{11}$	$= x_5 \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	K II
$\mathbf{B}_{12}$	$= -x_5 \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	K II
$\mathbf{B}_{13}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	K II
$\mathbf{B}_{14}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{19}$	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{y}}$	(8i)	O III
$\mathbf{B}_{20}$	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}}$	(8i)	O III
$\mathbf{B}_{21}$	$= (y_6 + \frac{1}{2}) \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2$	$=$	$a(y_6 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{y}}$	(8i)	O III

$$\begin{aligned}
\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) &\text{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) &\text{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) &\text{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) &\text{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) &\text{O IV} \\
\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}} &(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}} &(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}} &(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}} &(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}} &(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}} &(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}} &(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}} &(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}} &(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}} &(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}} &(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}} &(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}} &(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}} &(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}} &(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}} &(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}} &(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}} &(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}} &(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}} &(8j) &\text{O V}
\end{aligned}$$

References

- [1] A. Magnéli, *The crystal structure of tetragonal potassium bronze*, Arkiv Kemi **1**, 213–221 (1949).
- [2] B. G. Hyde and M. O’Keeffe, *Relations between the $\text{DO}_9(\text{ReO}_3)$ structure type and some "bronze" and "tunnel" structures*, Acta Crystallogr. Sect. A **29**, 243–248 (1973), doi:10.1107/S056773947300063X.

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First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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.