Orthorhombic UMo_5O_{16} Structure: A6B16C_oP23_16_su_acjlp2u_d-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.

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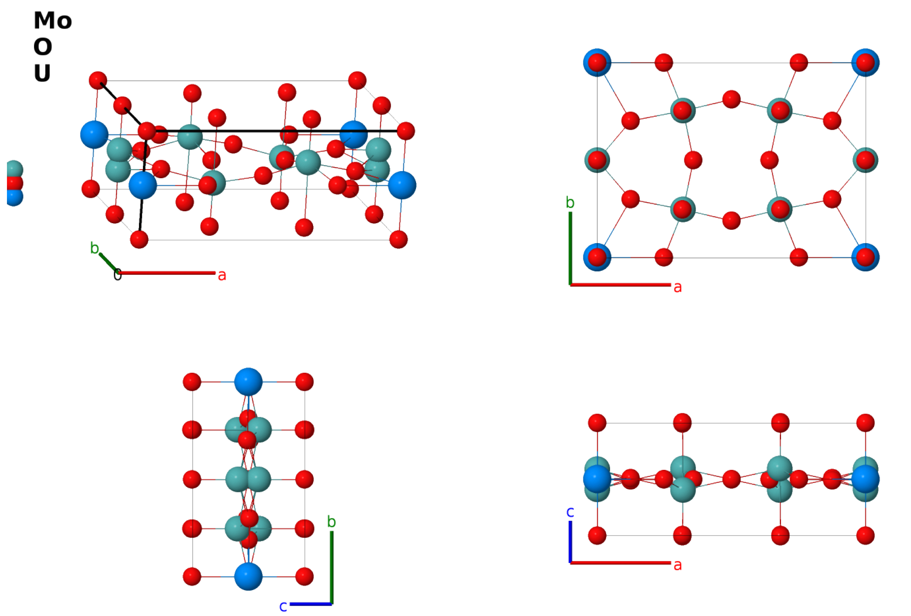
https://aflow.org/prototype-encyclopedia/CAAV

https://aflow.org/prototype-encyclopedia/A6B16C_oP23_16_su_acjlp2u_d-001



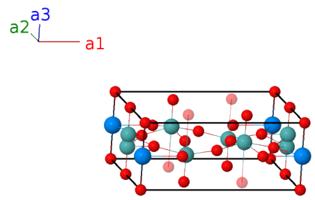
Prototype	$Mo_5O_{16}U$
AFLOW prototype label	A6B16C_oP23_16_su_acjlp2u_d-001
ICSD	80164
CCDC	1640388
Pearson symbol	oP23
Space group number	16
Space group symbol	$P222$
AFLOW prototype command	`aflow --proto=A6B16C_oP23_16_su_acjlp2u_d-001` `--params=`$a, b/a, c/a, x_4, x_5, y_6, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}$

- The Mo-I (2s) site is occupied only 50% of the time. For first-principles calculations it may be possible to replace the atoms on the (2s) site by a single atom at the (1g) site.
- (Tabachenko, 1995) also found evidence of a $U_{0.75}Mo_5O_{16}$ structure, where the uranium (1d) site contains 25% vacancies, and the Mo-II (4u) site is split into two partially occupied (4u) sites.

- (Tabachenko, 1995) also found a monoclinic UMo_5O_{16} structure, where the atoms are completely ordered.

Simple Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	U I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}b\,\hat{\mathbf{y}}$	(1c)	O I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(1g)	O II
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1$	=	$ax_4\,\hat{\mathbf{x}}$	(2i)	O III
$\mathbf{B_5}$	=	$-x_4\,\mathbf{a}_1$	=	$-ax_4\,\hat{\mathbf{x}}$	(2i)	O III
$\mathbf{B_6}$	=	$x_5\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2j)	O IV
$\mathbf{B_7}$	=	$-x_5\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2j)	O IV
$\mathbf{B_8}$	=	$y_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$by_6\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2n)	Mo I
$\mathbf{B_9}$	=	$-y_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-by_6\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2n)	Mo I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_7\,\hat{\mathbf{z}}$	(2r)	O V
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_7\,\hat{\mathbf{z}}$	(2r)	O V
$\mathbf{B_{12}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4u)	Mo II
$\mathbf{B_{13}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4u)	Mo II
$\mathbf{B_{14}}$	=	$-x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(4u)	Mo II
$\mathbf{B_{15}}$	=	$x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(4u)	Mo II
$\mathbf{B_{16}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(4u)	O VI
$\mathbf{B_{17}}$	=	$-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(4u)	O VI
$\mathbf{B_{18}}$	=	$-x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(4u)	O VI
$\mathbf{B_{19}}$	=	$x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(4u)	O VI
$\mathbf{B_{20}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(4u)	O VII
$\mathbf{B_{21}}$	=	$-x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(4u)	O VII
$\mathbf{B_{22}}$	=	$-x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}}$	(4u)	O VII
$\mathbf{B_{23}}$	=	$x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}}$	(4u)	O VII

References

[1] V. V. Tabachenko, O. G. D'yachenko, and M. Sundberg, *The crystal structures of UMo_5O_{16} and $U_{0.75}Mo_5O_{16}$ studies by X-ray diffraction and high resolution electron microscopy*, Eur. J. Solid State Inorg. Chem. **32**, 1137–1149 (1995).

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).