Monoclinic UMo_5O_{16} Structure: A5B16C_mP22_3_a2e_ab7e_b-001

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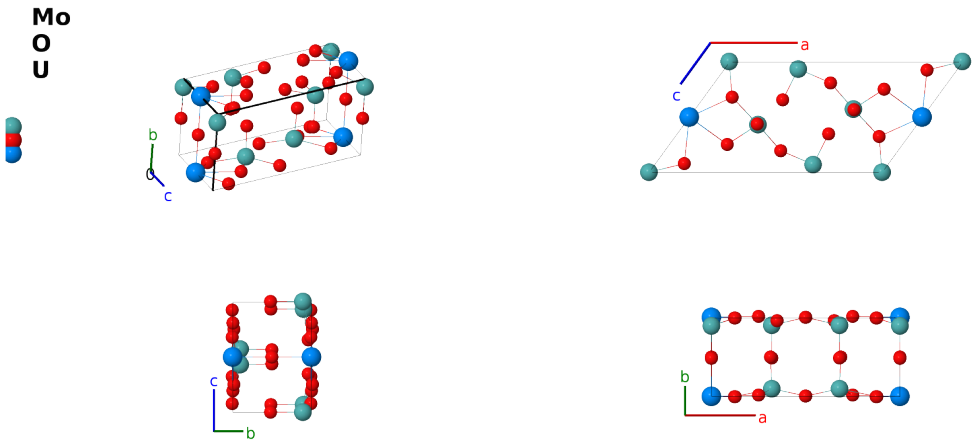
https://aflow.org/prototype-encyclopedia/LMET

https://aflow.org/prototype-encyclopedia/A5B16C_mP22_3_a2e_ab7e_b-001

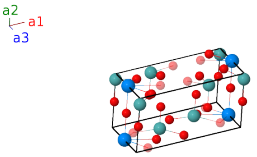


Prototype	$Mo_5O_{16}U$
AFLOW prototype label	A5B16C_mP22_3_a2e_ab7e_b-001
ICSD	80162
CCDC	1640386
Pearson symbol	mP22
Space group number	3
Space group symbol	$P2$
AFLOW prototype command	`aflow --proto=A5B16C_mP22_3_a2e_ab7e_b-001 --params=`$a, b/a, c/a, \beta, y_1, y_2, y_3, y_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}$

- (Tabachenko, 1995) also found an orthorhombic UMo_5O_{16} structure, where some of the molybdenum sites are disordered.
- (Tabachenko, 1995) give the data for this structure in the unique-axis c orientation of space group $P2$ #3. We used FINDSYM and AFLOW to transform this to the standard unique-axis b orientation. This makes substantial changes to the primitive vectors.
- Space group $P2$ allows an arbitrary choice of origin for the y-axis. Here we set y_4=0 for the uranium position.

Simple Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$y_1\,\mathbf{a}_2$	=	$by_1\,\hat{\mathbf{y}}$	(1a)	Mo I
$\mathbf{B_2}$	=	$y_2\,\mathbf{a}_2$	=	$by_2\,\hat{\mathbf{y}}$	(1a)	O I
$\mathbf{B_3}$	=	$y_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(1b)	O II
$\mathbf{B_4}$	=	$y_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(1b)	U I
$\mathbf{B_5}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(2e)	Mo II
$\mathbf{B_6}$	=	$-x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(2e)	Mo II
$\mathbf{B_7}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(2e)	Mo III
$\mathbf{B_8}$	=	$-x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(2e)	Mo III
$\mathbf{B_9}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(2e)	O III
$\mathbf{B_{10}}$	=	$-x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(2e)	O III
$\mathbf{B_{11}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(2e)	O IV
$\mathbf{B_{12}}$	=	$-x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(2e)	O IV
$\mathbf{B_{13}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(2e)	O V
$\mathbf{B_{14}}$	=	$-x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(2e)	O V
$\mathbf{B_{15}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(2e)	O VI
$\mathbf{B_{16}}$	=	$-x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(2e)	O VI
$\mathbf{B_{17}}$	=	$x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(2e)	O VII
$\mathbf{B_{18}}$	=	$-x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} - cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(2e)	O VII
$\mathbf{B_{19}}$	=	$x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(2e)	O VIII
$\mathbf{B_{20}}$	=	$-x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3$	=	$-(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} - cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(2e)	O VIII
$\mathbf{B_{21}}$	=	$x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$(ax_{13} + cz_{13}\cos\beta)\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + cz_{13}\sin\beta\,\hat{\mathbf{z}}$	(2e)	O IX
$\mathbf{B_{22}}$	=	$-x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3$	=	$-(ax_{13} + cz_{13}\cos\beta)\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} - cz_{13}\sin\beta\,\hat{\mathbf{z}}$	(2e)	O IX

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).

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