

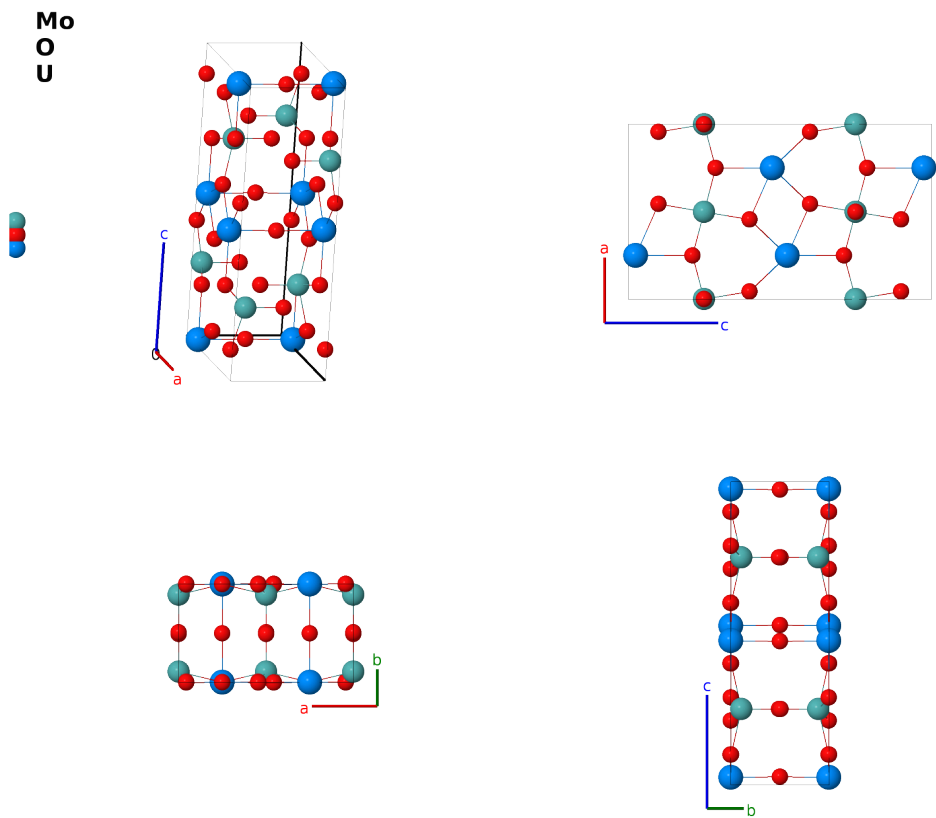
UMoO₅ Structure: AB5C_oP28_54_c_cdef_d-001

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<https://aflow.org/prototype-encyclopedia/3HAW>

https://aflow.org/prototype-encyclopedia/AB5C_oP28_54_c_cdef_d-001



Prototype	MoO ₅ U
AFLOW prototype label	AB5C_oP28_54_c_cdef_d-001
ICSD	82460
CCDC	1642545
Pearson symbol	oP28
Space group number	54
Space group symbol	<i>Pcca</i>
AFLOW prototype command	<code>aflow --proto=AB5C_oP28_54_c_cdef_d-001</code> <code>--params=a, b/a, c/a, y₁, y₂, z₃, z₄, z₅, x₆, y₆, z₆</code>

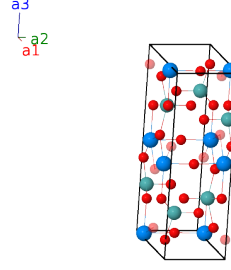
- (D'yachenko, 1996) present the structure in the *Pbaa* setting of space group #54. We used FINDSYM to transform this into the standard *Pcca* setting.

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
$\mathbf{B}_1$	$= y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	Mo I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	Mo I
$\mathbf{B}_3$	$= -y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	Mo I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	Mo I
$\mathbf{B}_5$	$= y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_7$	$= -y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_9$	$= \frac{1}{4} \mathbf{a}_1 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + cz_3 \hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B}_{10}$	$= \frac{3}{4} \mathbf{a}_1 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B}_{11}$	$= \frac{3}{4} \mathbf{a}_1 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - cz_3 \hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B}_{12}$	$= \frac{1}{4} \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B}_{13}$	$= \frac{1}{4} \mathbf{a}_1 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + cz_4 \hat{\mathbf{z}}$	(4d)	U I
$\mathbf{B}_{14}$	$= \frac{3}{4} \mathbf{a}_1 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	U I
$\mathbf{B}_{15}$	$= \frac{3}{4} \mathbf{a}_1 - z_4 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - cz_4 \hat{\mathbf{z}}$	(4d)	U I
$\mathbf{B}_{16}$	$= \frac{1}{4} \mathbf{a}_1 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	U I
$\mathbf{B}_{17}$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{18}$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{19}$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{20}$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B}_{21}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B}_{22}$	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B}_{23}$	$= -x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B}_{24}$	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B}_{25}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B}_{26}$	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 + y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8f)	O IV

$$\mathbf{B}_{27} = x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 = ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (8f) \quad \text{O IV}$$

$$\mathbf{B}_{28} = -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + y_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 = -a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (8f) \quad \text{O IV}$$

References

- [1] O. G. D'yachenko, V. V. Tabachenko, R. Tali, L. M. Kovba, B.-O. Marinder, and M. Sundberg, *Structure of UMoO_5 studied by single-crystal X-ray diffraction and high-resolution transmission electron microscopy*, Acta Crystallogr. Sect. B **52**, 961–965 (1996), doi:10.1107/S0108768196009597.

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