Na_4UO_5 Structure: A4B5C_tI20_87_h_ah_b-001

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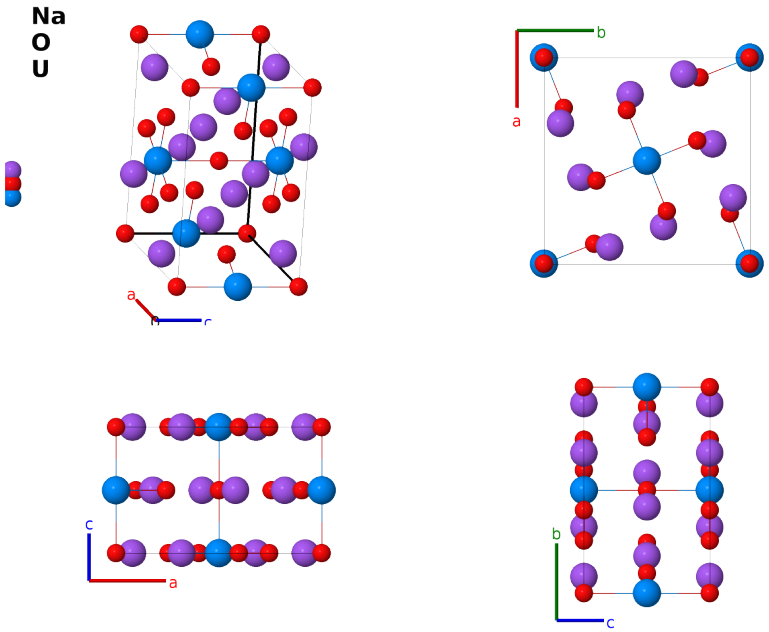
https://aflow.org/prototype-encyclopedia/N6CF

https://aflow.org/prototype-encyclopedia/A4B5C_tI20_87_h_ah_b-001

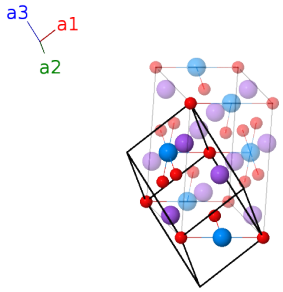


Prototype	Na_4O_5U
AFLOW prototype label	A4B5C_tI20_87_h_ah_b-001
ICSD	22203
CCDC	1598983
Pearson symbol	tI20
Space group number	87
Space group symbol	$I4/m$
AFLOW prototype command	`aflow --proto=A4B5C_tI20_87_h_ah_b-001 --params=`$a, c/a, x_3, y_3, x_4, y_4$

Other compounds with this structure
Li_4NpO_5, Li_4UO_5, Na_4NpO_5, Na_4PuO_5

Body-centered Tetragonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	O I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	U I
$\mathbf{B_3}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + (x_3+y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}}$	(8h)	Na I
$\mathbf{B_4}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - (x_3+y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}}$	(8h)	Na I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + (x_3-y_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(8h)	Na I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - (x_3-y_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(8h)	Na I
$\mathbf{B_7}$	=	$y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + (x_4+y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_8}$	=	$-y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - (x_4+y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + (x_4-y_4)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - (x_4-y_4)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(8h)	O II

References

[1] H. Hoekstra and S. Siegel, *Structural studies on Li_4UO_5 and Na_4UO_5*, J. Inorg. Nucl. Chem. **26**, 693–700 (1964), doi:10.1016/0022-1902(64)80311-0.

Found in

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