Weeksite ($USiO_7$) Structure: A7BC_oC36_38_3d2f_d_d-001

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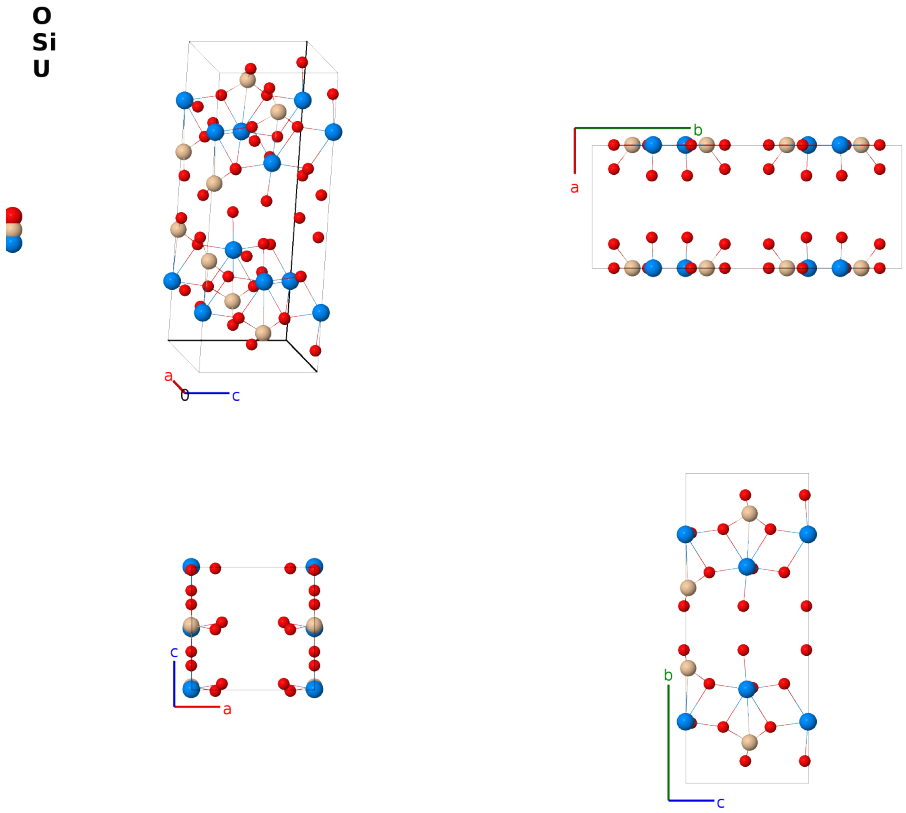
https://aflow.org/prototype-encyclopedia/8HLE

https://aflow.org/prototype-encyclopedia/A7BC_oC36_38_3d2f_d_d-001

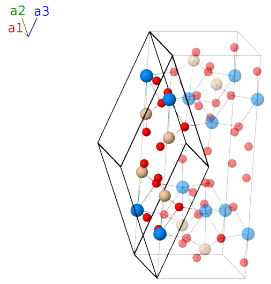


Prototype	O_7SiU
AFLOW prototype label	A7BC_oC36_38_3d2f_d_d-001
Mineral name	weeksite
ICSD	100771
CCDC	1659876
Pearson symbol	oC36
Space group number	38
Space group symbol	$Amm2$
AFLOW prototype command	`aflow --proto=A7BC_oC36_38_3d2f_d_d-001 --params=`$a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3, y_4, z_4, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

- (Stohl, 1981) call this a pseudocell of the actual structure, which is twice the size of this cell in all directions, however they were unable to determine the space group or atomic positions for that structure.
- Space group $Amm2$ #38 allows an arbitrary placement of the origin of the z-axis. Here $z_5 = 0$ for the uranium (2d) site.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$(y_1 - z_1)\,\mathbf{a}_2 + (y_1 + z_1)\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4d)	O I
$\mathbf{B_2}$	=	$-(y_1 + z_1)\,\mathbf{a}_2 - (y_1 - z_1)\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4d)	O I
$\mathbf{B_3}$	=	$(y_2 - z_2)\,\mathbf{a}_2 + (y_2 + z_2)\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B_4}$	=	$-(y_2 + z_2)\,\mathbf{a}_2 - (y_2 - z_2)\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B_5}$	=	$(y_3 - z_3)\,\mathbf{a}_2 + (y_3 + z_3)\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4d)	O III
$\mathbf{B_6}$	=	$-(y_3 + z_3)\,\mathbf{a}_2 - (y_3 - z_3)\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4d)	O III
$\mathbf{B_7}$	=	$(y_4 - z_4)\,\mathbf{a}_2 + (y_4 + z_4)\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4d)	Si I
$\mathbf{B_8}$	=	$-(y_4 + z_4)\,\mathbf{a}_2 - (y_4 - z_4)\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4d)	Si I
$\mathbf{B_9}$	=	$(y_5 - z_5)\,\mathbf{a}_2 + (y_5 + z_5)\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4d)	U I
$\mathbf{B_{10}}$	=	$-(y_5 + z_5)\,\mathbf{a}_2 - (y_5 - z_5)\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4d)	U I
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a}_1 + (y_6 - z_6)\,\mathbf{a}_2 + (y_6 + z_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{12}}$	=	$-x_6\,\mathbf{a}_1 - (y_6 + z_6)\,\mathbf{a}_2 - (y_6 - z_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{13}}$	=	$x_6\,\mathbf{a}_1 - (y_6 + z_6)\,\mathbf{a}_2 - (y_6 - z_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{14}}$	=	$-x_6\,\mathbf{a}_1 + (y_6 - z_6)\,\mathbf{a}_2 + (y_6 + z_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{15}}$	=	$x_7\,\mathbf{a}_1 + (y_7 - z_7)\,\mathbf{a}_2 + (y_7 + z_7)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{16}}$	=	$-x_7\,\mathbf{a}_1 - (y_7 + z_7)\,\mathbf{a}_2 - (y_7 - z_7)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{17}}$	=	$x_7\,\mathbf{a}_1 - (y_7 + z_7)\,\mathbf{a}_2 - (y_7 - z_7)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8f)	O V
$\mathbf{B_{18}}$	=	$-x_7\,\mathbf{a}_1 + (y_7 - z_7)\,\mathbf{a}_2 + (y_7 + z_7)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8f)	O V

References

[1] F. V. Stohl and D. K. Smith, *The crystal chemistry of the uranyl silicate minerals*, Am. Mineral. **66**, 610–625 (1981).

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

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