α-SiU_3 ($D0_c$) Structure: AB3_tI16_140_b_ah-001

This structure originally had the label `AB3_tI16_140_b_ah`. Calls to that address will be redirected here.

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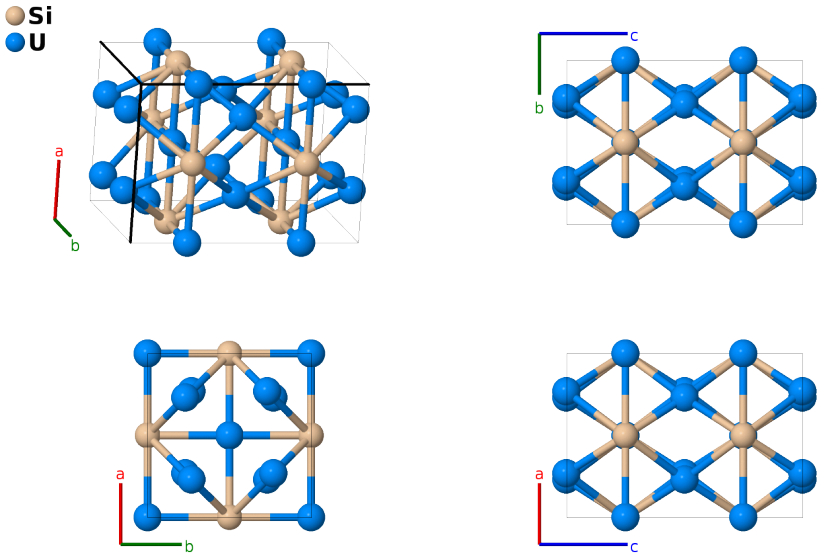
https://aflow.org/p/6CWC

https://aflow.org/p/AB3_tI16_140_b_ah-001



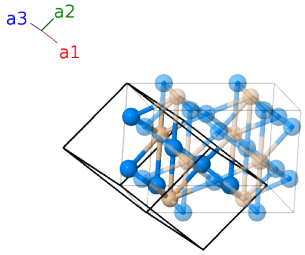
Prototype	SiU_3
AFLOW prototype label	AB3_tI16_140_b_ah-001
***Strukturbericht* designation**	$D0_c$
ICSD	31627
Pearson symbol	tI16
Space group number	140
Space group symbol	$I4/mcm$
AFLOW prototype command	`aflow --proto=AB3_tI16_140_b_ah-001 --params=`$a, c/a, x_3$

Other compounds with this structure
$AlPt_3$, $GaPt_3$, $GePt_3$, $SiIr_3$, $SiPt_3$ (HT)

- This is the ground state of SiU_3. Above 770°C it transforms into β-SiU_3 in the Cu_3Au ($L1_2$) structure. (Okamoto, 2013).
- When $c = 2a$ and $x_3 = 1/4$ the atoms are at the positions of the Cu_3Au ($L1_2$) structure.
- Many references define both a $D0_c$ and a $D0_c'$ (Ir_3Si) structure. The primary difference seems to be positioning the Si atoms on the (2a) or (2b) sites. Since this is merely an origin shift we will ignore the $D0_c'$ label.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\tfrac{1}{4}\,\mathbf{a}_1 + \tfrac{1}{4}\,\mathbf{a}_2$	=	$\tfrac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	U I
$\mathbf{B_2}$	=	$\tfrac{3}{4}\,\mathbf{a}_1 + \tfrac{3}{4}\,\mathbf{a}_2$	=	$\tfrac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	U I
$\mathbf{B_3}$	=	$\tfrac{3}{4}\,\mathbf{a}_1 + \tfrac{1}{4}\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	Si I
$\mathbf{B_4}$	=	$\tfrac{1}{4}\,\mathbf{a}_1 + \tfrac{3}{4}\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	Si I
$\mathbf{B_5}$	=	$\left(x_3 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(2x_3 + \tfrac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	U II
$\mathbf{B_6}$	=	$-\left(x_3 - \tfrac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(2x_3 - \tfrac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	U II
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 - \left(x_3 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(8h)	U II
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(8h)	U II

References

[1] W. H. Zachariasen, *Crystal chemical studies of the 5f-series of elements. VIII. Crystal structure studies of uranium silicides and of $CeSi_2$, $NpSi_2$, and $PuSi_2$*, Acta Cryst. **2**, 94–99 (1949), doi:10.1107/S0365110X49000217.

[2] H. Okamoto, *Si-U (Silicon-Uranium)*, J. Phase Equilibria Diffus. **34**, 167–168 (2013).