

α -SiU₃ ($D0_c$) Structure: AB3_tI16_140_b_ah-001

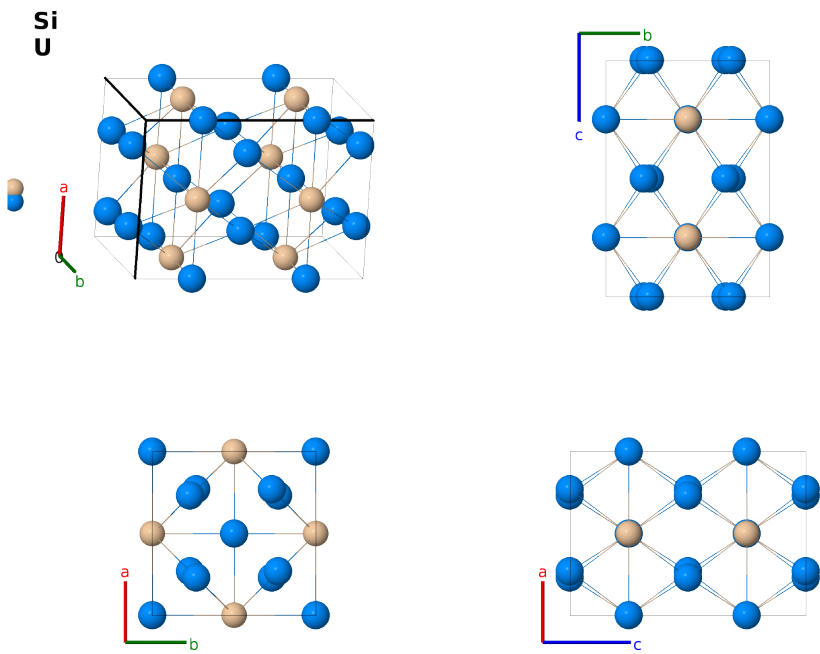
This structure previously used the label(s) **AB3-tI16.140.b_ah**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/6CWC>

https://aflow.org/prototype-encyclopedia/AB3_tI16_140_b_ah-001



Prototype	SiU ₃
AFLOW prototype label	AB3_tI16_140_b_ah-001
<i>Strukturbericht</i> designation	$D0_c$
ICSD	31627
CCDC	1605634
Pearson symbol	tI16
Space group number	140
Space group symbol	$I4/mcm$
AFLOW prototype command	<code>aflow --proto=AB3_tI16_140_b_ah-001</code> <code>--params=a, c/a, x₃</code>

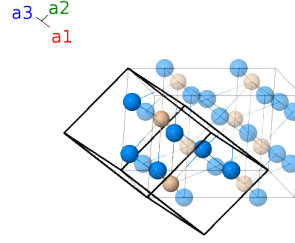
Other compounds with this structure

AlPt₃, GaPt₃, GePt₃, SiIr₃, SiPt₃ (HT)

- This is the ground state of SiU₃. Above 770°C it transforms into β -SiU₃ in the Cu₃Au (*L*₁₂) structure. (Okamoto, 2013).
 - When $c = 2a$ and $x_3 = 1/4$ the atoms are at the positions of the Cu₃Au (*L*₁₂) structure.
 - Many references define both a $D0_c$ and a $D0'_c$ (Ir₃Si) 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.
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Body-centered Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(4a)	U I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(4a)	U I
$\mathbf{B}_3$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4b)	Si I
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4b)	Si I
$\mathbf{B}_5$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 + (2x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	U II
$\mathbf{B}_6$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 - (2x_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	U II
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}}$	(8h)	U II
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}}$	(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 CeSi₂, NpSi₂, and PuSi₂*, 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).

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