Si_2U_3 ($D5_a$) Structure: A2B3_tP10_127_g_ah-001

This structure originally had the label `A2B3_tP10_127_g_ah`. Calls to that address will be redirected here.

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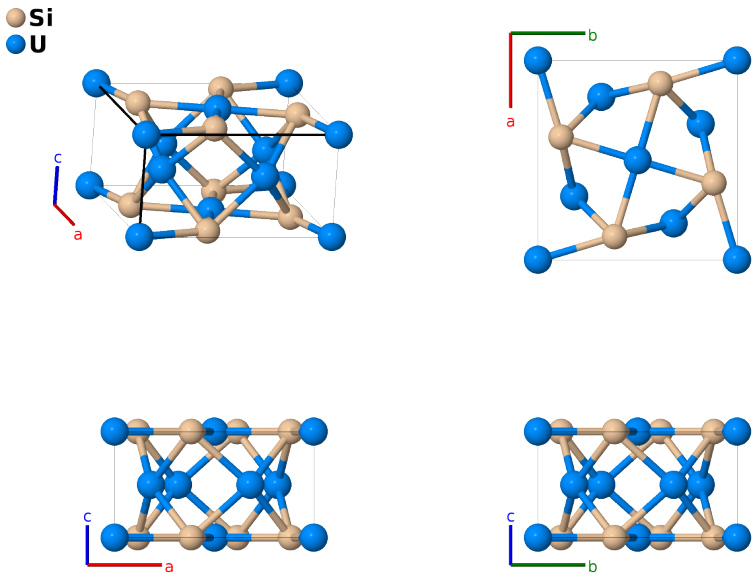
https://aflow.org/p/6QGS

https://aflow.org/p/A2B3_tP10_127_g_ah-001



Prototype	Si_2U_3
AFLOW prototype label	A2B3_tP10_127_g_ah-001
***Strukturbericht* designation**	$D5_a$
ICSD	73695
Pearson symbol	tP10
Space group number	127
Space group symbol	$P4/mbm$
AFLOW prototype command	`aflow --proto=A2B3_tP10_127_g_ah-001 --params=`$a, c/a, x_2, x_3$

Other compounds with this structure

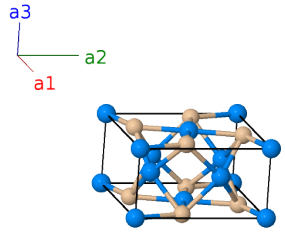
Al_2Th_3, B_2Mo_3, B_2Nb_3, B_2Ta_3, B_2V_3, Be_2Nb_3, Be_2Ta_3, Ga_2Nb_3, Ga_2Ta_3, Ga_2Zr_3, Ge_2Th_3, Pd_2Dy_3, Pd_2Ho_3, Si_2Hf_3, Si_2Th_3, Si_2Zr_3

- If we consider the Si_2 dimers as a pseudo-atom then this is a tetragonal distortion of the Cu_3Au ($L1_2$) structure.
- Mo_2FeB_2 is the ternary form of this structure.

- We use the lattice constants taken by (Remsching, 1992) at 1200°C, while the ICSD entry uses what are apparently the room temperature values.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	U I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(2a)	U I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	Si I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	Si I
$\mathbf{B_5}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(4g)	Si I
$\mathbf{B_6}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(4g)	Si I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	U II
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	U II
$\mathbf{B_9}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	U II
$\mathbf{B_{10}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	U II

References

[1] K. Remschnig, T. L. Bihan, H. Noël, and P. Rogl, *Structural chemistry and magnetic behavior of binary uranium silicides*, J. Solid State Chem. **97**, 391–399 (1992), doi:10.1016/0022-4596(92)90048-Z.

Found in

[1] P. Villars, K. Cenzual, R. Gladyshevskii, O. Shcherban, V. Dubenskyy, V. Kuprysyuk, I. Savesyuk, and R. Zaremba, *Landolt-Börnstein - Group III Condensed Matter* (2012). URL http://materials.springer.com/lb/docs/sm_lbs_978-3-642-22847-6_359.