α-$ThSi_2$ (C_c) Structure: A2B_tI12_141_e_a-002

This structure previously used the label(s) `A2B_tI12_141_e_a.ThSi2`. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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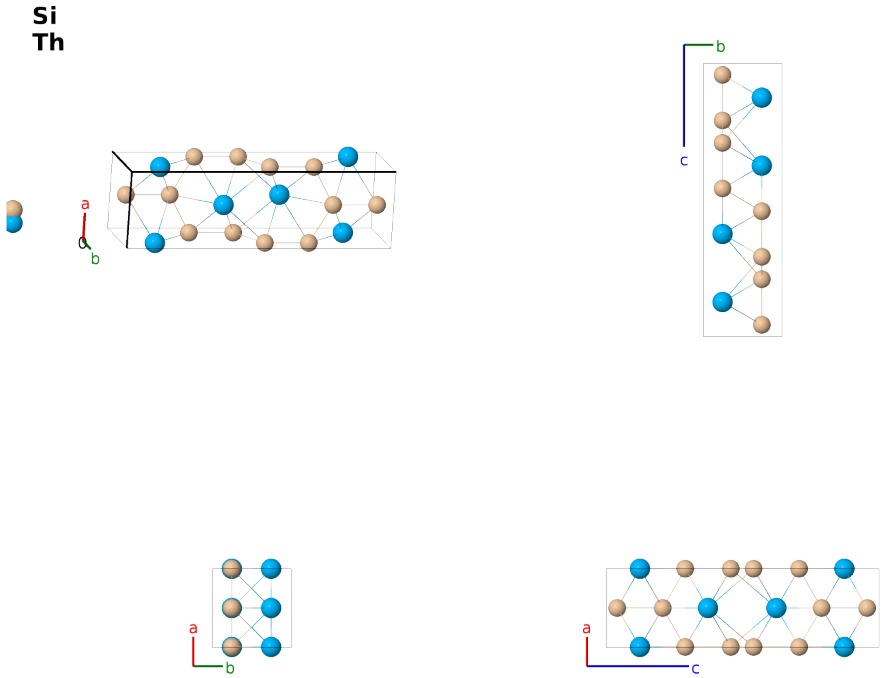
https://aflow.org/prototype-encyclopedia/NF8F

https://aflow.org/prototype-encyclopedia/A2B_tI12_141_e_a-002



Prototype	$ThSi_2$
AFLOW prototype label	A2B_tI12_141_e_a-002
***Strukturbericht* designation**	C_c
ICSD	77320
CCDC	1637759
Pearson symbol	tI12
Space group number	141
Space group symbol	$I4_1/amd$

AFLOW prototype command `aflow --proto=A2B_tI12_141_e_a-002 --params=`$a, c/a, z_2$

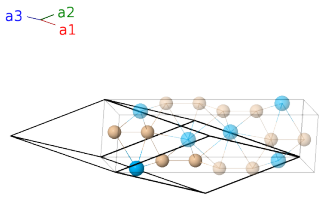
Other compounds with this structure

$CdSi_2$, $DySi_2$, $GdGe_2$, $LaGe_2$, $LaSi_2$, $NdGe_2$, $NpSi_2$, $PrGe_2$, $PuGe_2$, $PuSi_2$, $SmGe_2$, α-USi_2

- (Brauer, 1942) give the atomic positions in setting 1 of space group $I4_1/amd$ #141. AFLOW transforms this to the standard setting 2.
- Anatase TiO_2 ($C5$), α-$ThSi_2$ (C_c), and β-Mo_2N share the same AFLOW prototype label, A2B_tI12_141_e_a. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(4a)	Th I
$\mathbf{B_2}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(4a)	Th I
$\mathbf{B_3}$	=	$\left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8e)	Si I
$\mathbf{B_4}$	=	$z_2\,\mathbf{a}_1 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8e)	Si I
$\mathbf{B_5}$	=	$-\left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8e)	Si I
$\mathbf{B_6}$	=	$-z_2\,\mathbf{a}_1 - \left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8e)	Si I

References

[1] G. Brauer and A. Mitius, *Die Kristallstruktur des Thoriumsilicids $ThSi_2$*, Z. Anorganische und Allgemeine Chemie **249**, 325–339 (1942), doi:10.1002/zaac.19422490401.

Found in

[1] W. B. Pearson, *The Crystal Chemistry and Physics of Metals and Alloys* (Wiley Interscience, New York, London, Sydney, Tornoto, 1972).

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043