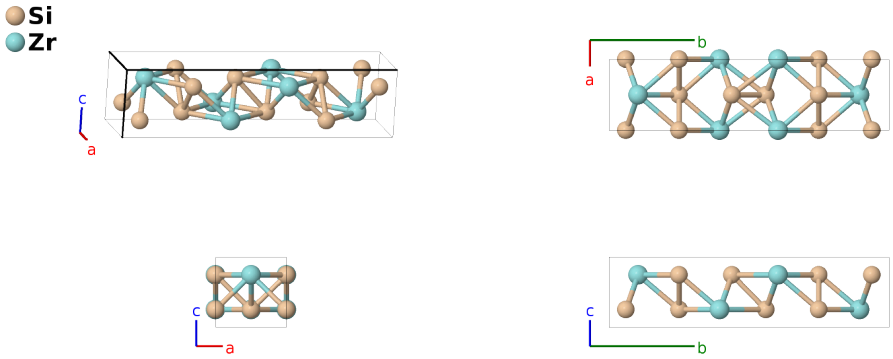
$ZrSi_2$ ($C49$) Structure: A2B_oC12_63_2c_c-001

This structure originally had the label `A2B_oC12_63_2c_c`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/HPCM

https://aflow.org/p/A2B_oC12_63_2c_c-001



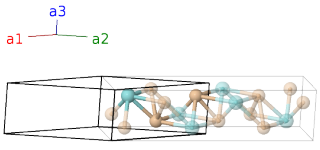
Prototype	Si_2Zr
AFLOW prototype label	A2B_oC12_63_2c_c-001
***Strukturbericht* designation**	$C49$
ICSD	652610
Pearson symbol	oC12
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=A2B_oC12_63_2c_c-001 --params=`$a, b/a, c/a, y_1, y_2, y_3$

Other compounds with this structure

Bi_2Ca, Bi_2Eu, Ge_2Hf, Ge_2Th, Ge_2U, Ge_2Zr, Si_2Hf, Si_2Ti, Sn_2Er, Sn_2Dy, Sn_2Gd, Sn_2Ho, Sn_2Lu, Sn_2Tb, Sn_2Tm, Sn_2Y, Sn_2Yb

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Si II
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Si II
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Zr I
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Zr I

References

[1] P. G. Cotter, J. A. Kohn, and R. A. Potter, *Physical and X-Ray Study of the Disilicides of Titanium, Zirconium, and Hafnium*, J. Am. Ceram. Soc. **39**, 11–12 (1956), doi:10.1111/j.1151-2916.1956.tb15590.x.

Found in

[1] P. Villars, *ZrSi2 Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.