$ZrFe_4Si_2$ Structure: A4B2C_tP14_136_i_f_a-001

This structure originally had the label `A4B2C_tP14_136_i_g_b`. Calls to that address will be redirected here.

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https://aflow.org/p/U6YK

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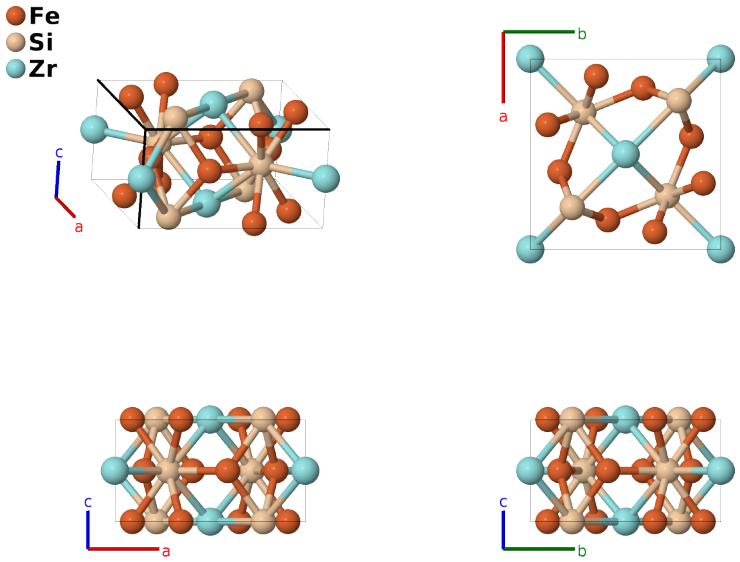


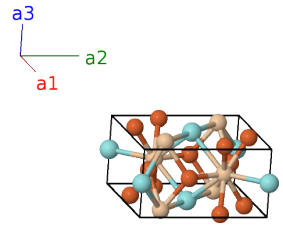
Prototype	Fe_4Si_2Zr
AFLOW prototype label	A4B2C_tP14_136_i_f_a-001
ICSD	87172
Pearson symbol	tP14
Space group number	136
Space group symbol	$P4_2/mnm$
AFLOW prototype command	`aflow --proto=A4B2C_tP14_136_i_f_a-001 --params=`$a, c/a, x_2, x_3, y_3$

Other compounds with this structure

$BaCd_4Pt_2$, $DyFe_4Ge_2$, $DyNi_4As_2$, $ErFe_4Ge_2$, $ErNi_4P_2$, $GdNi_4As_2$, $GdRe_4Si_2$, $HoFe_4Ge_2$, $LuFe_4Ge_2$, $LuNi_4As_2$, $LuRe_4Si_2$, $ScFe_4P_2$, $ScFe_4Si_2$, $ScNi_4As_2$, $SmRe_4Si_2$, $SrCd_4Pt_2$, $TbRe_4Si_2$, $TmFe_4Ge_2$, $TmRe_4Si_2$, UMn_4P_2, YFe_4Ge_2, YNi_4As_2, YNi_4P_2, YRe_4Si_2, $YbNi_4P_2$, $ZrFe_4P_2$, $ZrNi_4As_2$

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)	Zr I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Zr I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(4f)	Si I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(4f)	Si I
$\mathbf{B_5}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4f)	Si I
$\mathbf{B_6}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4f)	Si I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}}$	(8i)	Fe I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}}$	(8i)	Fe I
$\mathbf{B_9}$	=	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8i)	Fe I
$\mathbf{B_{10}}$	=	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8i)	Fe I
$\mathbf{B_{11}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8i)	Fe I
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8i)	Fe I
$\mathbf{B_{13}}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(8i)	Fe I
$\mathbf{B_{14}}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(8i)	Fe I

References

[1] Y. P. Yarmolyuk, L. A. Lysenko, and E. I. Gladyshevsky, *Crystal Structure of $ZrFe_4Si_2$ – A New Structure Type of Ternary Silicides*, Dopov. Akad. Nauk Ukr. RSR, Ser. A **37**, 281–284 (1975). In Russian.

Found in

[1] P. Schobinger-Papamantellos, J. Rodrıguez-Carvajal, G. André, N. P. Duong, K. H. J. Buschow, and P. Tolédano, *Simultaneous structural and magnetic transitions in YFe_4Ge_2 studied by neutron diffraction and magnetic measurements*, J. Magn. Magn. Mater. **236**, 14–27 (2001), doi:10.1016/S0304-8853(01)00442-5.