TiFeSi Structure: ABC_oI36_46_ac_bc_3b-001

This structure previously used the label(s) `ABC_oI36_46_ac_bc_3b`. Calls to these addresses will be redirected here.

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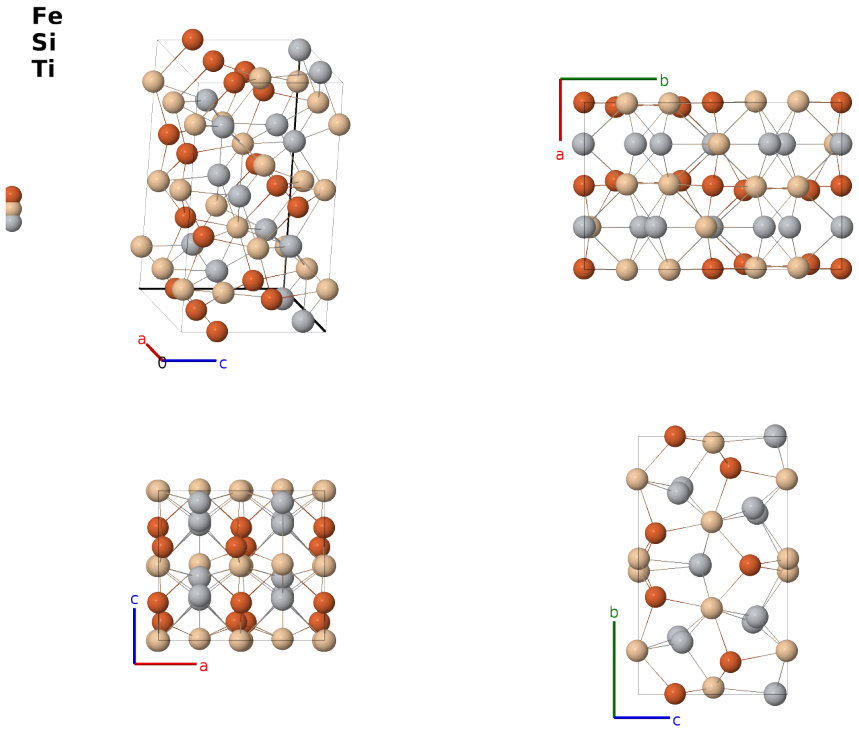
https://aflow.org/prototype-encyclopedia/7FJR

https://aflow.org/prototype-encyclopedia/ABC_oI36_46_ac_bc_3b-001



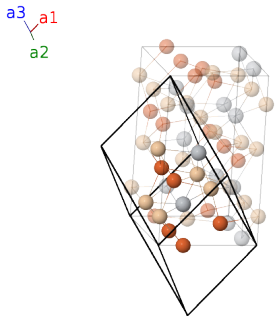
Prototype	FeSiTi
AFLOW prototype label	ABC_oI36_46_ac_bc_3b-001
ICSD	41157
CCDC	1610954
Pearson symbol	oI36
Space group number	46
Space group symbol	$Ima2$
AFLOW prototype command	`aflow --proto=ABC_oI36_46_ac_bc_3b-001 --params=`$a, b/a, c/a, z_1, y_2, z_2, y_3, z_3, y_4, z_4, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

Other compounds with this structure

DyMnGa, ErMnGa, FeNbGe, GdMnGa, HfOsSi, HfRuAs, HfRuSi, HoMnGa, NbReSi, NbRuSi, TaReSi, TaRuSi, TiIrSi, TiOsGe, TiOsSi, TiRhGe, TiRuAs, TiRuGe, RhMnGe, RuTiSi, RuZrGe, TaMnGe, TaMnSi, TbMnGa, TiFeGe, YMnGa

Body-centered Orthorhombic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(4a)	Fe I
$\mathbf{B_2}$	=	$z_1\,\mathbf{a}_1 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_1\,\hat{\mathbf{z}}$	(4a)	Fe I
$\mathbf{B_3}$	=	$(y_2 + z_2)\,\mathbf{a}_1 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4b)	Si I
$\mathbf{B_4}$	=	$-(y_2 - z_2)\,\mathbf{a}_1 + \left(z_2 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4b)	Si I
$\mathbf{B_5}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + \left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	Ti I
$\mathbf{B_6}$	=	$-(y_3 - z_3)\,\mathbf{a}_1 + \left(z_3 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(y_3 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	Ti I
$\mathbf{B_7}$	=	$(y_4 + z_4)\,\mathbf{a}_1 + \left(z_4 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_4 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4b)	Ti II
$\mathbf{B_8}$	=	$-(y_4 - z_4)\,\mathbf{a}_1 + \left(z_4 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(y_4 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4b)	Ti II
$\mathbf{B_9}$	=	$(y_5 + z_5)\,\mathbf{a}_1 + \left(z_5 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_5 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4b)	Ti III
$\mathbf{B_{10}}$	=	$-(y_5 - z_5)\,\mathbf{a}_1 + \left(z_5 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(y_5 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4b)	Ti III
$\mathbf{B_{11}}$	=	$(y_6 + z_6)\,\mathbf{a}_1 + (x_6 + z_6)\,\mathbf{a}_2 + (x_6 + y_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	Fe II
$\mathbf{B_{12}}$	=	$-(y_6 - z_6)\,\mathbf{a}_1 - (x_6 - z_6)\,\mathbf{a}_2 - (x_6 + y_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	Fe II
$\mathbf{B_{13}}$	=	$-(y_6 - z_6)\,\mathbf{a}_1 + \left(x_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_6 - y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	Fe II
$\mathbf{B_{14}}$	=	$(y_6 + z_6)\,\mathbf{a}_1 + \left(-x_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_6 + y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	Fe II

$\mathbf{B_{15}}$	$=$	$(y_7 + z_7)\ \mathbf{a}_1 + (x_7 + z_7)\ \mathbf{a}_2 + (x_7 + y_7)\ \mathbf{a}_3$	$=$	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8c)	Si II
$\mathbf{B_{16}}$	$=$	$-(y_7 - z_7)\ \mathbf{a}_1 - (x_7 - z_7)\ \mathbf{a}_2 - (x_7 + y_7)\ \mathbf{a}_3$	$=$	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8c)	Si II
$\mathbf{B_{17}}$	$=$	$-(y_7 - z_7)\ \mathbf{a}_1 + \left(x_7 + z_7 + \frac{1}{2}\right)\ \mathbf{a}_2 + \left(x_7 - y_7 + \frac{1}{2}\right)\ \mathbf{a}_3$	$=$	$a\left(x_7 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8c)	Si II
$\mathbf{B_{18}}$	$=$	$(y_7 + z_7)\ \mathbf{a}_1 + \left(-x_7 + z_7 + \frac{1}{2}\right)\ \mathbf{a}_2 + \left(-x_7 + y_7 + \frac{1}{2}\right)\ \mathbf{a}_3$	$=$	$-a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8c)	Si II

References

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[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

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